A scaling approach to the theory of magnetic Kondo lattices

1992 J. Phys.: Condens. Matter 4 9661

(http://iopscience.iop.org/0953-8984/4/48/020)

A scaling approach to the theory of magnetic Kondo lattices

V Yu Irkhin and M I Katsnelson
Institute of Metal Physics, 620219 Ekaterinburg, Russia

Received 6 May 1992

Abstract. A scaling consideration of the magnetically ordered state in concentrated Kondo lattices is carried out within the periodic s–f exchange model. Renormalization-group equations for the effective s–f parameter and spin-fluctuation frequency are derived taking account of the influence of intersite exchange interactions on the Kondo effect in paramagnetic, ferromagnetic and antiferromagnetic states. Depending on the relation between the one-impurity Kondo temperature T_K and the bare spin-fluctuation frequency $\overline{\omega}$, three regimes are possible: (i) the strong coupling regime where all the conduction electrons are bound into singlet states, which occurs at $\overline{\omega} < T_K$; (ii) the regime of a 'Kondo' magnet with an appreciable, but not total, compensation of magnetic moments, at $T_K < \overline{\omega} < AT_K$, $A \gtrsim 1$; and (iii) the regime of 'usual' magnets with small logarithmic corrections to $\overline{\omega}$ and saturation magnetic moment $\overline{S}$, at $\overline{\omega} \gg T_K$. In the case of the ferromagnetic s–f exchange interaction, explicit expressions for the renormalizations of $\overline{S}$ and $\overline{\omega}$ are obtained.

1. Introduction

Experimental investigations over the last few years have convincingly demonstrated that magnetic ordering is widespread among heavy-fermion systems and other anomalous 4f and 5f compounds, which are treated as concentrated Kondo systems. There exist numerous examples of systems ($CeRh_3B_2$, $CeAl_2$, TmS, CeB_6, $UAgCu_4$, YbNiSn) where 'Kondo' anomalies in thermodynamic and transport properties coexist with magnetic ordering, the saturation moment M_s being of the order of $1\mu_B$. As for heavy-fermion systems themselves, the situation is more complicated. There exists unambiguous evidence for antiferromagnetic ordering in UCd_{11} and U_2Zn_{17} with the same order of magnitude as M_s [1]. For UPt_3, $M_s \simeq 2 \times 10^{-2}\mu_B$ [2]. Antiferromagnetic ordering with very small M_s was also reported for $CeAl_3$ [3], UBe_{13} [4] and $CeCu_2Si_2$ [5]. However, the data for $CeAl_3$ and UBe_{13}, respectively, were not confirmed in [6, 7]. Generally, a characteristic feature of heavy-fermion magnets is high sensitivity of M_s to external factors such as pressure and doping by a small amount of impurities. So, UBe_{13} becomes an antiferromagnet with an appreciable M_s under a pressure $P > 23$ kbar; on the contrary, $CeAl_3$ becomes paramagnetic above $P = 3$ kbar [8]. The moment in UPt_3 increases up to values of the order of $1\mu_B$ upon adding 5% of Pd instead of Pt, or Th instead of U [9]. These exotic properties of Kondo magnets have stimulated a number of attempts at their theoretical explanation [10–15]. However, results of various approaches are contradictory. In the present paper we treat the problem of magnetic Kondo lattices using a simple scaling consideration within the s–f exchange model.

0953-8984/92/489661+12$07.50

Specifics of Kondo magnets are determined by the competition between spin dynamics due to intrasite interactions among f spins (with a characteristic scale $\overline{\omega}$) and the intersite Kondo effect characterized by the Kondo temperature T_K. At $T > T_K$ the 'Kondo' logarithms in perturbation corrections to various physical quantities are smeared: $\ln T \to \frac{1}{2}\ln(T^2 + \overline{\omega}^2)$ [10], the quantity $\overline{\omega}$ itself decreasing on lowering T. A hypothesis was put forward in [11] that a unified energy scale $\overline{\omega}(T < T_K) \sim T_K$ is established. This hypothesis is based on experimental data on magnetic neutron scattering in dense Kondo systems: the width of the quasi-elastic peak is of the same order of magnitude as the Fermi degeneracy temperature determined from thermodynamic and transport properties. In the framework of such a picture, the Kondo compensation of magnetic moments on lowering T stops at $T \sim T_K$, which results in the formation of a state with small but finite M_s. Here we consider the conditions for the occurrence of this regime as functions of bare values of T_K and $\overline{\omega}$.

In sections 2 and 3 we derive the system of scaling equations for the effective s–f interaction, spin dynamics frequency and magnetic moment in various magnetic phases. In section 4 we investigate these equations to obtain explicit estimations for the magnetic characteristics. In section 5 we discuss the applicability of the results obtained to real f systems.

2. Effective s–f interaction in Kondo lattices

We proceed with the Hamiltonian of the periodic s–f exchange model

$$H = \sum_{k,\sigma} \epsilon_k c^{+}_{k\sigma} c_{k\sigma} - I \sum_{kq\alpha\beta} \sigma_{\alpha\beta} S_q c^{+}_{k+q,\alpha} c_{k\beta} - \sum_q J_q S_q S_{-q} \tag{1}$$

where $c^{+}_{k\sigma}$ are the creation operators for conduction electrons with quasi-momentum k and spin projection σ, ϵ_k is the band energy referred to the chemical potential, S_q are the Fourier components of the spin-density operators for the f subsystem, σ are the Pauli matrices, I is the s–f exchange parameter, and J_q are the Fourier transforms of the 'direct' f–f exchange integrals J_R. As a rule, in real anomalous rare-earth compounds, J_R are nothing but RKKY (Ruderman–Kittel–Kasuya–Yoshida) indirect exchange parameters. However, when constructing perturbation theory in I, it is convenient to consider J_q as independent parameters and include the last term in (1) in the zero-order Hamiltonian. We apply the 'poor man scaling' approach by Anderson [16], who considered the case of one Kondo impurity. To this end we divide the space of conduction-electron states into layers with energies $C < E < C + \delta C$ and calculate the contribution of each layer to the effective s–f parameter $I_{ef}(C)$. In the case of the lattice of interacting f spins, the latter is defined in a different way in comparison with the one-impurity situation. Moreover, the definitions are slightly different for the paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AFM) phases.

To determine $I_{ef}(E)$ in these three cases, we calculate the self-energy Σ of the retarded anticommutator Green function

$$G_{k\sigma}(E) = \langle\langle c_{k\sigma} \mid c^{+}_{k\sigma}\rangle\rangle_E = [E - \epsilon_k - \Sigma_{k\sigma}(E)]^{-1}. \tag{2}$$

First we consider the simplest FM case. Using the Holstein–Primakoff representation for spin operators,

$$\begin{aligned} S^{+}_i &= \sqrt{2}S\left\{1 - [1/(2S)]b^{+}_i b_i\right\}^{1/2} b_i \\ S^{-}_i &= \sqrt{2}S b^{+}_i \left\{1 - [1/(2S)]b^{+}_i b_i\right\}^{1/2} \qquad S^z_i = S - b^{+}_i b_i \end{aligned} \tag{3}$$

we obtain at $T = 0$ to second order in I the well known expressions (see e.g. [10])

$$\Sigma_{k\uparrow}(E) = -IS + 2I^2 S \sum_q \frac{f_{k+q,\downarrow}}{E - \epsilon_{k+q,\downarrow} + \omega_q} \tag{4a}$$

$$\Sigma_{k\downarrow}(E) = IS + 2I^2 S \sum_q \frac{1 - f_{k-q,\uparrow}}{E - \epsilon_{k-q,\uparrow} - \omega_q} \tag{4b}$$

where $\omega_q = 2S(J_0 - J_q) \simeq Dq^2$ is the magnon frequency, $f_{k\sigma} = f(\epsilon_{k\sigma})$ is the Fermi distribution function, $\epsilon_{k\uparrow,\downarrow} = \epsilon_k \mp IS$. The many-electron second-order terms in (4) yield logarithmic corrections at $E \to 0$, which are cut at the magnon energies. It is natural to define the quantity I_{ef} in terms of the spin splitting of the conduction electron at the Fermi level

$$\Sigma_{k\downarrow}(E) - \Sigma_{k\uparrow}(E) = 2I_{\text{ef}}S \qquad k = k_{\text{F}}, E = 0. \tag{5}$$

Then the contribution of intermediate electron states with energies $C < \epsilon_{k+q,-\sigma} < C + \delta C$ in (4) is given by

$$\delta I_{\text{ef}}(C) = I^2 \sum_{C<\epsilon_{k+q,\uparrow}<C+\delta C} \frac{1}{\epsilon_{k+q,\uparrow} + \omega_q} + I^2 \sum_{C<\epsilon_{k+q,\downarrow}<C+\delta C} \frac{1}{\epsilon_{k+q,\downarrow} - \omega_q}$$
$$\simeq (\rho I^2/\overline{\omega})\delta C \ln((C - \overline{\omega})/(C + \overline{\omega})) \tag{6}$$

where $\overline{\omega} = 4Dk_{\text{F}}^2$, and ρ is the density of states at the Fermi level. For $\overline{\omega} \to 0$ we obtain from (6)

$$\delta I_{\text{ef}}(C) = -(2\rho I^2/C)\delta C \tag{7}$$

which coincides with the result in the case of one impurity, obtained in [16] for a different definition of I_{ef}. Making in $\partial I_{\text{ef}}/\partial C$ the replacements $I \to I_{\text{ef}}(C)$, $\overline{\omega} \to \overline{\omega}_{\text{ef}}(C)$ and introducing the dimensionless coupling constant

$$g = -2I\rho \qquad g_{\text{ef}}(C) = -2I_{\text{ef}}(C)\rho \tag{8}$$

we obtain the renormalization-group equation

$$\partial g_{\text{ef}}(C)/\partial C = (g_{\text{ef}}^2(C)/2\overline{\omega}_{\text{ef}}(C)) \ln((C + \overline{\omega}_{\text{ef}}(C))/(C - \overline{\omega}_{\text{ef}}(C))). \tag{9}$$

The dependence $\overline{\omega}_{\text{ef}}(C)$ arises due to many-electron corrections to the magnon frequency. The second scaling equation determining $\overline{\omega}_{\text{ef}}(C)$ will be obtained in the next section. Now we consider the AFM case. As demonstrated in [10], unlike the FM situation, Kondo-like contributions to the self-energy arise in the third order in I, since the leading contribution of the AFM gap to the electron spectrum is of order I^2. It is convenient to use the matrix representation including the longitudinal (in the local coordinate system) part of the s–f interaction, which describes the formation of the AFM gap, in the zero-order Hamiltonian. Passing to the magnon representation, we rewrite the Hamiltonian (1) in the form

$$H = H_0 + H_{\text{int}} \tag{10}$$

$$H_0 = \sum_k \psi_k^+ E_k \psi_k + \sum_q \omega_q \alpha_q^+ \alpha_q \tag{11}$$

$$H_{\text{int}} = \sum_{kq} \psi_k^+ W_q \psi_{k+q} \tag{12}$$

where $\psi_k^+ = (c_{k\uparrow}^+, c_{k+Q,\downarrow}^+)$ are the spinor Fermi operators, α_q^+ are the magnon creation operators, Q is the wavevector of the AFM structure (we put for simplicity $2Q = G$ with G being a reciprocal-lattice vector),

$$E_k = \begin{pmatrix} \epsilon_k & -IS \\ -IS & \epsilon_{k+Q} \end{pmatrix} = \tfrac{1}{2}(\epsilon_k + \epsilon_{k+Q}) + \tfrac{1}{2}(\epsilon_k - \epsilon_{k+Q})\sigma_z - IS\sigma_x \tag{13}$$

is the zero-order electron energy matrix,

$$W_q = I(S/2)^{1/2}\left[(u_q - v_q)(\alpha_{-q}^+ + \alpha_q)\sigma_z - \mathrm{i}(u_q + v_q)(\alpha_{-q}^+ - \alpha_q)\sigma_y\right] \tag{14}$$

is the operator of the electron–magnon interaction, and u_q and v_q are the coefficients of the Bogoliubov transformation diagonalizing the f–f interaction Hamiltonian,

$$\left\{ \begin{matrix} u_q^2 \\ v_q^2 \end{matrix} \right\} = \tfrac{1}{2}\left(S\frac{2J_Q - J_{Q+q} - J_q}{\omega_q} \pm 1 \right) \tag{15}$$

$$\omega_q^2 = 4S^2(J_Q - J_q)(J_Q - J_{Q+q}). \tag{16}$$

To obtain the many-electron Kondo contributions, it is sufficient to calculate the matrix self-energy defined by

$$\langle\langle \psi_k \mid \psi_k^+ \rangle\rangle_E = [E - E_k - \Sigma(k, E)]^{-1} \tag{17}$$

to second order in W_q. Using the diagram technique in the Matsubara representation, we derive

$$\begin{aligned} \Sigma(k, \mathrm{i}\epsilon_n) = \frac{I^2 S}{2} T \sum_{q, \mathrm{i}\omega_m} \frac{2\omega_q}{\omega_m^2 + \omega_q^2} [\mathrm{i}\epsilon_n - \mathrm{i}\omega_m - E_1(k-q)]^{-1} [\mathrm{i}\epsilon_n - \mathrm{i}\omega_m - E_2(k-q)]^{-1} \\ \times \{(u_q - v_q)^2 \sigma_z [\mathrm{i}\epsilon_n - \mathrm{i}\omega_m - \tfrac{1}{2}(\epsilon_{k-q} + \epsilon_{k+Q-q}) \\ + \tfrac{1}{2}(\epsilon_{k-q} - \epsilon_{k+Q-q})\sigma_z - IS\sigma_x]\sigma_z \\ + (u_q + v_q)^2 \sigma_y [\mathrm{i}\epsilon_n - \mathrm{i}\omega_m - \tfrac{1}{2}(\epsilon_{k-q} + \epsilon_{k+Q-q}) \\ + \tfrac{1}{2}(\epsilon_{k-q} - \epsilon_{k+Q-q})\sigma_z - IS\sigma_x]\sigma_y\} \end{aligned} \tag{18}$$

where $\epsilon_n = (2n+1)\pi T$, $\omega_m = 2m\pi T$, $m, n = 0, \pm 1, \ldots$ and

$$E_{1,2}(k) = \tfrac{1}{2}(\epsilon_k + \epsilon_{k+Q}) \pm [\tfrac{1}{4}(\epsilon_k - \epsilon_{k+Q})^2 + I^2 S^2]^{1/2} \tag{19}$$

is the electron spectrum in the mean-field approximation. We assume that the 'nesting' condition $\epsilon_{k+Q} = -\epsilon_k$ is not satisfied, so that the AFM gap does not destroy the Fermi surface. Then we may put in (18) $E_1(k) \simeq \epsilon_k$, $E_2(k) \simeq \epsilon_{k+Q}$. To determine I_{ef} we have to calculate the term in (18) that is proportional to σ_x (this renormalizes the AFM gap):

$$I_{\mathrm{ef}} = I - (1/S)\Sigma_x(k, E)|_{\epsilon_k = E = 0}. \tag{20}$$

Such a definition is equivalent to that for a ferromagnet (5). Calculating the sum over ω_m, retaining only contributions with the Fermi functions and performing the analytical continuation $\mathrm{i}\epsilon_n \to E + \mathrm{i}0$, we derive

$$\begin{aligned} \Sigma_x(k, E) = -I^2 S \sum_q f_{k-q}(E - \epsilon_{k-q}) \\ \times \left(1/[\omega_q^2 - (E - \epsilon_{k-q})^2] + 1/[\omega_{q+Q}^2 - (E - \epsilon_{k-q})^2]\right). \end{aligned} \tag{21}$$

When taking into account spin dynamics, the space dimension turns out, unlike the usual Kondo effect, to be important. We consider two-dimensional and three-dimensional cases. The former may be relevant to the current carriers in copper oxide planes of high-T_c superconductors and parent compounds (e.g. in the antiferromagnet $Pr_{1-x}Y_xBa_2Cu_3O_7$ with large electronic specific heat [17]). Calculating the integral in (21) in the approximation $\omega_q = \omega_{q+Q} = v_a q$ (v_a is the antiferromagnon velocity) and introducing the coupling constant (8), we derive

$$\frac{\partial g_{ef}(C)}{\partial C} = \begin{cases} g_{ef}^2(C)/[C^2 - \overline{\omega}_{ef}^2(C)]^{1/2} & \text{2D} \\ -[g_{ef}^2(C)C/\overline{\omega}_{ef}^2(C)]\ln[1 - \overline{\omega}_{ef}^2(C)/C^2] & \text{3D} \end{cases} \qquad (22)$$

with the bare value $\overline{\omega} = 2v_a k_F$. In the paramagnetic phase the s–f interaction results in the occurrence of electron damping, which is determined by Im $\Sigma_k(E)$, rather than of spectrum spin splitting. In the third order of perturbation theory in I we obtain the Kondo singular corrections [10], which differ from those for one impurity by the replacement

$$\sum_p \frac{f_p}{E - \epsilon_p} \to \int_{-\infty}^{\infty} d\omega \sum_p K_{p-k}(\omega) \frac{f_p}{E - \epsilon_p + \omega} \qquad (23)$$

where $K_q(\omega)$ is the spectral density of the Green function for interacting f spins, normalized to unity. The correction δI_{ef} is found from the renormalization of I in the second-order expression for the damping by the Kondo third-order contribution. If we adopt the spin diffusion approximation

$$K_q(\omega) = (1/\pi) D_s q^2 / [\omega^2 + (D_s q^2)^2] \qquad (24)$$

with $D_s \sim JS^2$ the spin diffusion constant, we obtain the equation for the coupling constant in the 3D case

$$\frac{\partial g_{ef}(C)}{\partial C} = \mathrm{Re}\left[\frac{g_{ef}^2(C)}{i\overline{\omega}_{ef}(C)} \ln\left(1 + \frac{i\overline{\omega}_{ef}(C)}{C}\right)\right] = g_{ef}^2(C)\frac{\tan^{-1}[\overline{\omega}_{ef}(C)/C]}{\overline{\omega}_{ef}(C)} \qquad (25)$$

the characteristic spin diffusion frequency $i\overline{\omega} = 4iD_s k_F^2$ being purely imaginary (spin dynamics is dissipative).

In all cases the renormalization-group equation may be represented in the form

$$\partial g_{ef}(C)/\partial C = (g_{ef}^2(C)/C)\phi(\overline{\omega}_{ef}(C)/C) \qquad (26)$$

where the explicit form of the function ϕ depends on the type of magnetic ordering and space dimension:

$$\phi(x) = \begin{cases} [1/(2x)]\ln[(1+x)/(1-x)] & \text{3D FM} \\ (1-x^2)^{-1/2} & \text{2D AFM} \\ -(1/x^2)\ln(1-x^2) & \text{3D AFM} \\ (1/x)\tan^{-1} x & \text{3D PM.} \end{cases} \qquad (27)$$

Note that the condition $\phi(0) = 1$, which guarantees the correct limit of one Kondo impurity [16], is satisfied. It is interesting that there is no essential difference between FM, AFM and PM phases in terms of g_{ef}.

3. Renormalization of spin dynamics frequencies

The problem of spin-fluctuation frequency renormalization in the PM phase was considered in [11]. The mean square of the frequency was determined from the second moment of the spin Green function

$$\langle\omega_q^2\rangle = (\dot{S}_q^z, \dot{S}_{-q}^z)/(S_q^z, S_{-q}^z) \tag{28}$$

$$(A, B) = \int_0^\beta \mathrm{d}\lambda\, \langle \mathrm{e}^{\lambda H} A \mathrm{e}^{-\lambda H} B\rangle. \tag{29}$$

To second order in I one obtains

$$\langle\omega_q^2\rangle = \langle\omega_q^2\rangle_{I=0}[1 - 4I^2(1-\alpha_q)L] \tag{30}$$

$$L = \sum_{pq} \frac{f_p(1-f_q)}{(\epsilon_p - \epsilon_q)^2} \simeq \rho^2 \ln\left(\frac{W}{T}\right) \tag{31}$$

where W is of the order of the conduction band width, and

$$\alpha_q = \sum_R J_R^2 \left(\frac{\sin(k_\mathrm{F} R)}{k_\mathrm{F} R}\right)^2 [1 - \cos(qR)] \Big/ \sum_R J_R^2[1-\cos(qR)] \tag{32}$$

is a function of q with values $0 < \alpha_q < 1$. In the nearest-neighbour approximation for J_R, α does not depend on q:

$$\alpha_q \equiv \alpha = [\sin(k_\mathrm{F} d)/k_\mathrm{F} d]^2 \tag{33}$$

where d is the distance between nearest neighbours. If one takes into account the cutting of the Kondo divergence at spin-fluctuation frequencies, expression (31) is replaced by

$$L = \int_{-\infty}^{\infty} \mathrm{d}\omega \sum_{pq} \frac{f_p(1-f_q)}{(\epsilon_p - \epsilon_q + \omega)^2} K_{p-q}(\omega) \tag{34}$$

which yields in the diffusion approximation (24)

$$L = \sum_{pq} \frac{f_p(1-f_q)}{(\epsilon_p - \epsilon_q)^2 + \overline{\omega}^2} \qquad \overline{\omega} = 4D_\mathrm{s} k_\mathrm{F}^2. \tag{35}$$

Substituting (35) into (30), picking out the contributions from the layers with occupied electron states with $C < \epsilon_p < C + \delta C$ and introducing the coupling constant (8), we obtain the scaling equation for $\overline{\omega}_\mathrm{ef}(C)$

$$\partial \ln \overline{\omega}_\mathrm{ef}(C)/\partial C = -[(1-\alpha)/2C] g_\mathrm{ef}^2(C) \phi(\overline{\omega}_\mathrm{ef}(C)/C) \tag{36}$$

with the same function $\phi(x)$ as in (25) and (27). Consider the case of a ferromagnet. To obtain the leading (in I) many-electron correction to the magnon frequency, one has to perform in the equation of motion for the magnon Green function

$$\omega\langle\langle b_q \mid b_q^+\rangle\rangle_\omega = 1 + \langle\langle [b_q, H] \mid b_q^+\rangle\rangle_\omega \tag{37}$$

commutation with the Heisenberg f–f Hamiltonian only. Using (3) the latter may be represented to first order in $1/S$ in the form

$$H_{\rm f} = 2S\sum_q (J_0 - J_q) b_q^+ b_q + \tfrac{1}{2}\sum_{qpr}(J_q + J_r - 2J_{q-r}) b_q^+ b_p^+ b_r b_{q+p-r}. \tag{38}$$

Then we obtain for the magnon pole the standard result

$$\omega_q = 2S(J_0 - J_q) + 2\sum_p (J_p + J_q - J_{p-q} - J_0)\langle b_p^+ b_p\rangle \tag{39}$$

which takes into account the magnon–magnon interaction. The magnon occupation numbers contain the zero-point contributions, which arise through the finite damping $\gamma_p(\omega)$ due to electron–magnon interaction [10]:

$$\delta\langle b_p^+ b_p\rangle = -\frac{1}{\pi}\int_{-\infty}^{0} \frac{{\rm d}\omega\,\gamma_p(\omega)}{(\omega - \omega_p)^2 + \gamma_p^2(\omega)} \simeq 2I^2 S\sum_k \frac{f_{k\downarrow}(1 - f_{k+p,\uparrow})}{(\epsilon_{k\downarrow} - \epsilon_{k+p,\uparrow} - \omega_p)^2}. \tag{40}$$

Substituting (40) into (39), picking out the contribution from the layer with $C < \epsilon_{k\downarrow} < C + \delta C$, carrying out the integration in the nearest-neighbour approximation and summing over q, we obtain the same result (36).

Finally for the AFM phase we have (cf [10])

$$\omega_q^2 = C_q^2 - D_q^2 \tag{41}$$

$$C_q = S(2J_Q - J_{Q+q} - J_q) - \sum_p (2J_Q + 2J_{Q+q-p} - J_p - J_q - J_{Q+p} - J_{Q+q})\langle b_p^+ b_p\rangle - \sum_p (J_{Q+p} - J_p)\langle b_p b_{-p}\rangle \tag{42}$$

$$D_q = S(J_{Q+q} - J_q) - \sum_p (J_{Q+q} + J_{Q+p} - J_q - J_p)\langle b_p^+ b_p\rangle + \sum_p (J_{Q+p} + J_p)\langle b_p b_{-p}\rangle \tag{43}$$

where b_p^+ are creation operators for spin deviations in the local coordinate system. We obtain similar to (40) (see [10])

$$\delta\left\{\begin{array}{c}\langle b_p^+ b_p\rangle\\ \langle b_p b_{-p}\rangle\end{array}\right\} = I^2 S\sum_k\left(\frac{f_k(1 - f_{k-p})}{(\epsilon_k - \epsilon_{k-p})^2 - \omega_p^2} \pm \frac{f_k(1 - f_{Q+k-p})}{(\epsilon_k - \epsilon_{k+Q-p})^2 - \omega_p^2}\right). \tag{44}$$

In the nearest-neighbour approximation where $J_{q+Q} = -J_q$ we derive

$$\delta\omega_q^2 = -4I^2(1-\alpha)\omega_q^2\sum_{kp}\frac{f_k(1 - f_{k-p})}{(\epsilon_k - \epsilon_{k-p})^2 - \omega_p^2} \tag{45}$$

where the constant α is given by (33). Then we have again the result (36) with the corresponding choice of the function $\phi(x)$ in (27). In the same way we may obtain the renormalization-group equation for the magnetic moment. In the PM phase this is determined from the Curie constant in the static magnetic susceptibility

$$\chi(T) = C(T)/T \qquad C(T) = \overline{S}_{\rm ef}^2(T)/3 \tag{46}$$

and in the FM and AFM phases by

$$\overline{S}_{\rm ef} = S - \sum_p \langle b_p^+ b_p\rangle. \tag{47}$$

Taking into account the 'Kondo' corrections to χ [10] and magnon occupation numbers (40) and (44), we obtain for all the phases

$$\partial\ln\overline{S}_{\rm ef}(C)/\partial C = (g_{\rm ef}^2(C)/C)\phi(\overline{\omega}_{\rm ef}(C)/C) \tag{48}$$

where the function ϕ is defined by the same equation (27).

4. Investigation of renormalization-group equations

The system of scaling equations obtained in previous sections may be represented as

$$\partial g_{\rm ef}(C)/\partial C = \Lambda \tag{49}$$

$$\partial \ln \overline{\omega}_{\rm ef}(C)/\partial C = -\tfrac{1}{2}(1-\alpha)\Lambda \tag{50}$$

$$\partial \ln \overline{S}_{\rm ef}(C)/\partial C = -\tfrac{1}{2}\Lambda \tag{51}$$

with

$$\Lambda = \Lambda(C, \overline{\omega}_{\rm ef}(C)) = (g^2_{\rm ef}(C)/C)\phi(\overline{\omega}_{\rm ef}(C)/C). \tag{52}$$

The first integral of the system (49), (50) reads

$$g_{\rm ef}(C) + [2/(1-\alpha)] \ln \overline{\omega}_{\rm ef}(C) = \text{constant} \tag{53}$$

which yields

$$\overline{\omega}_{\rm ef}(C) = \overline{\omega} \exp\left\{-\tfrac{1}{2}(1-\alpha)[g_{\rm ef}(C) - g]\right\} \tag{54}$$

where $\overline{\omega}$ is the bare characteristic spin-fluctuation energy (without Kondo renormalizations). Substituting (54) into (49) we obtain

$$\partial g_{\rm ef}/\partial \xi = g^2_{\rm ef}\Psi\left[\lambda + \tfrac{1}{2}(1-\alpha)g_{\rm ef} - \xi\right] \tag{55}$$

where

$$\Psi(x) = \phi({\rm e}^{-x}) \qquad \Psi(x \gg 1) = 1 \tag{56}$$

$$\xi = \ln|W/C| \qquad \lambda = \ln|W/\overline{\omega}| \gg 1 \tag{57}$$

and W is the cut-off energy of the order of the bandwidth, at which $g_{\rm ef}(C)$ coincides with the bare value g. Spin dynamics enters (56) via the parameter λ and the function Ψ. Consider the region where

$$\xi \ll \lambda + \tfrac{1}{2}(1-\alpha)g_{\rm ef}(\xi). \tag{58}$$

Then we may replace in (55) $\Psi(x)$ by unity to obtain

$$g_{\rm ef}(\xi) = g/(1-g\xi). \tag{59}$$

The inequality (58) holds in the region $\xi \ll \xi_1$ where ξ_1 is the minimal solution to the equation

$$\lambda + \tfrac{1}{2}(1-\alpha)g/(1-g\xi) = \xi. \tag{60}$$

At $\xi \simeq \xi_1$ the effective coupling constant $g_{\rm ef}(\xi)$ begins to deviate appreciably from the 'one-impurity' behaviour (59). To investigate the further evolution of $g_{\rm ef}$ one has to solve equation (55) explicitly. It is convenient to represent the latter in the form

$$1/g_{\rm ef}(\xi) = 1/g - X(\xi) \tag{61}$$

where

$$X(\xi) = \int_0^\xi {\rm d}\xi' \, \Psi(\lambda + \tfrac{1}{2}(1-\alpha)g_{\rm ef}(\xi') - \xi'). \tag{62}$$

Consider the 'Kondo' case $g > 0$ ($I < 0$). Since $\Psi(x)$ is a positive monotonically increasing function of x, it follows from (61) that $g_{\rm ef}(\xi)$ is a monotonically increasing function. Suppose that a fixed point with finite coupling constant exists, $g_{\rm ef}(\xi \to \infty) \to g^*$. Then

$$M(\lambda) < X(\infty) < M(\lambda + \tfrac{1}{2}(1-\alpha)g^*) \tag{63}$$

where

$$M(x) = \int_0^\infty \mathrm{d}\xi\, \Psi(x-\xi) = \int_{-\infty}^x \mathrm{d}\xi\, \Psi(\xi). \tag{64}$$

By virtue of (56) we may replace in (63) $M(x) \to x$ to obtain

$$\lambda g < 1 \qquad g^* < (2/g)(1-\lambda g)/(1-\alpha). \tag{65}$$

Thus at $\lambda g > 1$, i.e.

$$\overline{\omega} < T_{\rm K} \equiv W \exp(-1/g) \tag{66}$$

the supposition about finiteness of g^* leads to a contradiction, and there exists a point ξ^* where $g_{\rm ef}(\xi^*)$ diverges. Then (54) gives $\overline{\omega}_{\rm ef}(\xi^*) = 0$. As follows from the comparison of (50) and (51),

$$\overline{S}_{\rm ef}(\xi)/S = [\overline{\omega}_{\rm ef}(\xi)/\overline{\omega}]^{1/(1-\alpha)}. \tag{67}$$

Therefore $\overline{S}_{\rm ef}(\xi^*) = 0$ too. Detailed investigation of the true dependences $\overline{\omega}_{\rm ef}(\xi)$ and $\overline{S}_{\rm ef}(\xi)$ in this regime requires a scaling consideration beyond perturbation theory (e.g. by using the numerical renormalization-group technique). Qualitatively, a strong-coupling region with total compensation of the magnetic moment exists under condition (66), spin dynamics being totally suppressed. This case is relevant also for diluted Kondo systems where $\overline{\omega} \to 0$, $\lambda \to \infty$. We see that the Kondo divergences in such a situation may be cut at static magnetic fields only, but not at spin dynamics frequencies, which are renormalized to zero.

In the opposite case $\lambda g \ll 1$ we obtain from (60), (54) and (67)

$$\xi_1 \simeq \lambda + (1-\alpha)g \qquad g_{\rm ef}(\xi_1) \simeq g + \lambda g^2 \tag{68}$$

$$\overline{\omega}^* = \overline{\omega}_{\rm ef}(\xi_1) \simeq \overline{\omega}[1 - \tfrac{1}{2}(1-\alpha)\lambda g^2] \tag{69}$$

$$\overline{S}^* = \overline{S}_{\rm ef}(\xi_1) \simeq S(1 - \tfrac{1}{2}\lambda g^2). \tag{70}$$

At $\xi > \xi_1$ the increase of the coupling constant (see (59)) stops, and we obtain $X(\xi) \sim \lambda \ll 1/g$. Then (61) yields $g_{\rm ef} \simeq g$ at any ξ, so that the perturbation expressions (69) and (70) (cf [10]) are the final results in the regime under consideration, and we have the usual magnetic state.

As follows from the second inequality in (65), in the region

$$0 < 1 - \lambda g = \mathrm{O}(g) \qquad g \to 0 \tag{71}$$

one has $g^* = \mathrm{O}(1)$, $\overline{\omega}_{\rm ef}$ and $\overline{S}_{\rm ef}$ being renormalized several times. Thus the condition (71) determines the region of parameter values where the 'Kondo magnet' state with considerably suppressed, but finite, $\overline{S}_{\rm ef}$ and $\overline{\omega}_{\rm ef}$ occurs. In such a state, by virtue of (54), (65) and (67),

$$\overline{\omega}^* = \overline{\omega}_{\rm ef}(\xi = \infty) > T_{\rm K} \tag{72}$$

$$\overline{S}^* = \overline{S}_{\rm ef}(\xi = \infty) > S(T_{\rm K}/\overline{\omega})^{1/(1-\alpha)}. \tag{73}$$

Consider the case of the 'ferromagnetic' s–f exchange $I > 0$ ($g < 0$). Then, for $|g| \ll 1$, we have $|g_{ef}(\xi)| \ll 1$ at any ξ, and

$$X(\xi \to \infty) \simeq M(\lambda) \simeq \lambda. \tag{74}$$

Thus we can sum up the logarithmic divergences in all the orders of perturbation theory. Similar to (72) and (73) we obtain

$$g^* \simeq g/(1 - \lambda g) \tag{75}$$

$$\overline{\omega}^* = \overline{\omega} \exp[-\tfrac{1}{2}(1 - \alpha)\lambda g^2/(1 - \lambda g)] \tag{76}$$

$$\overline{S}^* = S \exp[-\tfrac{1}{2}\lambda g^2/(1 - \lambda g)]. \tag{77}$$

5. Discussion and conclusions

First we discuss the more simple case $I > 0$. This corresponds to the situation where the intra-atomic 'Hund' interaction dominates over the hybridization (Schrieffer–Wolff) contribution to the s–f interaction, and is apparently realized in 'usual' f magnets including elemental rare-earth metals (the hybridization contribution is small in the case where characteristics of f electrons are close to those in free atoms). Usually $|g|$ is small in such a situation (in rare-earth metals $|g| \sim 10^{-2}$). Then we may restrict ourselves to the second-order corrections [10]

$$\overline{S}^* \simeq S[1 - \tfrac{1}{2}g^2 \ln(W/\overline{\omega})] \tag{78}$$

$$\overline{\omega}^* \simeq \overline{\omega}[1 - \tfrac{1}{2}(1 - \alpha)g^2 \ln(W/\overline{\omega})]. \tag{79}$$

However, for diluted systems of both f and d elements, $\overline{\omega}$ may be small enough to satisfy the conditions $g\lambda \sim 1$ and even $g^2\lambda \sim 1$. Then we have to use the full expressions (76) and (77). At $|g| \ll 1$, but $|g|\lambda \gg 1$ the corrections to saturation magnetization and spin-dynamics frequencies are of the order of $|g|$.

Now we pass to the 'Kondo' case $I < 0$. Depending on the relation of T_K and $\overline{\omega}$, three cases are possible:

(i) $\overline{\omega} < T_K$. On approaching the Fermi level $C = 0$ (physically, with decreasing T), $\overline{\omega}_{ef}$ decreases so quickly that it cannot prevent entering the strong-coupling region $g_{ef}(\xi) = \infty$ and formation of the singlet non-magnetic state. The 'Kondo temperature' in the lattice is determined from the condition of divergence of g_{ef} at $E = T_K^*$. As follows from (61),

$$1/g = X(\ln W/T_K). \tag{80}$$

This quantity differs somewhat from the corresponding one-impurity value: $T_K^* < T_K$ since $X(\xi) < \xi$. This regime is relevant for diluted Kondo systems where $\overline{\omega} \to 0$ and for non-magnetic Kondo lattices (e.g., $CeCu_6$).

(ii) $T_K < \overline{\omega} < AT_K$ with $A \gtrsim 1$ (see equation (71)). A rather strong suppression of magnetic moment and spin dynamics takes place, but the ground state remains magnetic, the saturation moment increasing from zero to a quantity of order of μ_B with increasing $\overline{\omega}$. Apparently, this case corresponds to 'Kondo' and heavy-fermion magnetic systems. It is important that the magnetic moment may change strongly for small variations of the bare coupling constant g:

$$\delta g \sim g^2 \ll g \qquad g \sim 1/\ln(W/\overline{\omega}). \tag{81}$$

This explains qualitatively the high sensitivity of magnetic properties of heavy-fermion systems to doping and external pressure.

(iii) $\overline{\omega} \gg T_K$. This case corresponds to the usual ('non-Kondo') magnets with $I < 0$. It is sufficient here to take into account the second-order corrections (80).

Let us consider some questions concerning the applicability of the results obtained to real anomalous f systems.

Using the s–f exchange model (rather than, say, the Anderson-lattice model) in our consideration seems to be unimportant, since, for small coupling constants, the properties of the two models are similar.

Of course, intermediate valence systems cannot be treated within the s–f model. If we consider them as Kondo lattices with high T_K, we come to the conclusion that they should be, as a rule, non-magnetic. An important question is that about the nature of the 'Kondo' state with $g_{ef} \to \infty$ ($\xi \to \xi^*$). As follows from our consideration in the mean-field approximation for $T \ll T_K$ [11, 12], such a state may be ferromagnetic if the number of current carriers is smaller than that of localized spins. Thus, entering the strong-coupling region does not inevitably mean formation of singlet states on all the sites. However, in any case the peculiar 'Kondo' state is formed. In the mean-field approximation the latter is described by an order parameter corresponding to coupling (hybridization) of conduction electrons with f pseudo-fermions, the quasi-particle spectrum being of the same form as in the hybridization model with a characteristic energy scale T_K. The problem of magnetic properties of systems with such a spectrum needs further investigation. According to [11, 12], they are reminiscent of the properties of itinerant magnets with Stoner exchange parameter being replaced by intersite Heisenberg interaction. Of great interest are the heavy-fermion systems with a vanishing number of current carriers like Sm_3Se_4 [18] and $Yb_4As_{3-x}P_x$ [19]. A hypothesis was put forward in [20] that such systems possess a resonating valence bond (RVB) type state with Fermi excitations in the localized spin (or pseudo-spin) system. A scaling consideration of saturation moment renormalization and spin dynamics in such a situation would be instructive.

References

[1] Stewart G R 1984 *Rev. Mod. Phys.* **56** 755
[2] Aeppli G, Bucher F, Broholm C, Kjems J K, Baumann J and Hufnagl J 1988 *Phys. Rev. Lett.* **60** 615
[3] Nakamura H, Kitaoka Y, Asayama K and Floquet J 1988 *J. Phys. Soc. Japan* **57** 2644
[4] Kleiman R N, Bishop D J, Ott R H, Fisk Z and Smith J L 1990 *Phys. Rev. Lett.* **64** 1975
[5] Nakamura H, Kitaoka Y, Yamada H and Asayama K 1988 *J. Magn. Magn. Mater.* **76–77** 517
[6] Wong W H and Clark W G 1992 *J. Magn. Magn. Mater.* **108** 175
[7] de Visser A, van Dijk H, Franse J J M, Lacerda A, Floquet J, Fisk Z and Smith J L 1992 *J. Magn. Magn. Mater.* **108** 56
[8] Jaccard D, Sierro J, Brison J P and Floquet J 1988 *J. Physique Coll.* **49** C8 741
[9] Frings P, Renker B and Vettier C 1987 *J. Magn. Magn. Mater.* **63–64** 202
[10] Irkhin V Yu and Katsnelson M I 1989 *Z. Phys.* B **75** 67
Vonsovsky S V, Irkhin V Yu and Katsnelson M I 1990 *Physica* B **163** 321
[11] Irkhin V Yu and Katsnelson M I 1991 *Z. Phys.* B **82** 77

[12] Irkhin V Yu and Katsnelson M I 1990 *J. Phys.: Condens. Matter* **2** 8715
[13] Evans S M M 1991 *J. Phys.: Condens. Matter* **3** 8441
[14] Fazekas P and Mueller-Hartmann E 1991 *Z. Phys.* B **85** 285
[15] Coleman P 1990 *Physica* B **171** 3
[16] Anderson P W 1970 *J. Phys. C: Solid State Phys.* **3** 2346
[17] Kebede A, See C S, Schwegler J, Crow J E, Michalisin T, Myer G H, Salomon R E, Schlottmann P, Kurie M V, Bloom S H and Guertin R P 1989 *Phys. Rev.* B **40** 4453
[18] Fraas K, Ahlheim U, Reinders P H P, Schank C, Caspary R, Steglich F, Ochiai A, Suzuki T and Kasuya T 1992 *J. Magn. Magn. Mater.* **108** 220
[19] Nakamura O, Oyamada A, Ochiai A, Kunii S, Takeda T, Suzuki T and Kasuya T 1988 *J. Magn. Magn. Mater.* **76–77** 293
[20] Irkhin V Yu and Katsnelson M I 1990 *Phys. Lett.* **150A** 47