

The exact susceptibility of a Kondo spin- $1/2$  for ferromagnetic coupling and  $T=0$

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys.: Condens. Matter 2 3841

(<http://iopscience.iop.org/0953-8984/2/16/013>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.103

The article was downloaded on 11/05/2010 at 05:53

Please note that [terms and conditions apply](#).

# The exact susceptibility of a Kondo spin- $\frac{1}{2}$ for ferromagnetic coupling and $T = 0$

F Göhmann† and H Schulz

Institut für Theoretische Physik, Universität Hannover, Federal Republic of Germany

Received 31 August 1989, in final form 5 December 1989

**Abstract.** The magnetisation induced by a localised spin- $\frac{1}{2}$  interacting with the itinerant electrons of a paramagnetic host metal is obtained for a known band Kondo model and for the ‘other’ sign of coupling. Using the formal Bethe *ansatz* solution to this model the ground state energy is found for both the interacting host electrons and for the same system with impurity. The host magnetic properties are enhanced by a Stoner-like exchange. The impurity susceptibility diverges inverse-logarithmically at vanishing applied magnetic field—a result not accessible via perturbation theory.

## 1. Introduction

The magnetism of itinerant electrons and the magnetic properties of impurities imbedded in a host metal are typical areas of solid state theory where non-perturbative methods are required (Moriya 1985, 1987). The best non-perturbative method to apply to any problem is that of solving it exactly. Ten years ago, the purists succeeded by reactivating the Bethe *ansatz* and solved, e.g., the Kondo problem (Andrei *et al* 1983, Tsvetick and Wiegmann 1983). If one uses the Bethe *ansatz* one is far from ‘applying a method’. Instead there are only very few Hamiltonians that have Bethe-type eigenstates. Thus the construction of such a model is the crux of the matter. If this has been achieved, whether the model has reasonable overlap with physical reality depends on a further lucky accident. This paper is based on such an event.

Consider a magnetic impurity (modelled by a spin- $\frac{1}{2}$  localised at the origin) in contact with the band electrons of a paramagnetic host metal. Due to the repulsive e–e interaction in the bulk there will be exchange enhancement above the value of the Pauli susceptibility. If the half spin couples ferromagnetically, one expects the formation of an additional magnetisation cloud around the impurity (at least at non-zero applied magnetic field). This picture might apply to very dilute alloys the band electrons of which couple ferromagnetically to the magnetic ions (contained, e.g., Fe ions in the ppm range in a Rh host). The question arises as to how the corresponding excess magnetisation due to the impurity varies with the applied field. Here we shall concentrate on this question, and we shall give the exact answer. But the answer, as might be admitted, refers to a model, and (inevitably) a model is specialised.

In a previous paper (Schulz 1987—henceforth referred to as I) the following band Kondo Hamiltonian was proposed to overcome certain cut-off difficulties with the

† Present address: Physikalisches Institut der Universität Bayreuth, D-8580 Bayreuth, Federal Republic of Germany.

already existing 'relativistic' Kondo model (Wiegmann 1980, 1981, Andrei 1980), but without losing exact solvability. In I the formal solution was worked out and studied for antiferromagnetic coupling ( $g < 0$ ) until the Kondo effect was obtained. Here, however, we consider the case of ferromagnetic coupling  $g > 0$

$$H = \int_0^\infty dk k^2 c_{ka}^\dagger c_{ka} - \frac{2g}{\pi} \int_0^\infty dk \int_0^\infty dk' c_{ka}^\dagger [\tau \sigma_{ab} + (1-w)\delta_{ab}] c_{k'b} + H_{\text{int}}. \quad (1)$$

The first term in (1) is the s-wave part of the kinetic energy of the band electrons. The energy scale is such that  $\hbar^2/2m = 1$ . Only the s-wave states  $\sin(kr)/r$  couple to a pointlike impurity.  $a, b$  are spin indices (sum convention).  $\tau$  is the Pauli spin matrix vector of the impurity.  $g$  is a matrix element taken out of the integrals after neglecting all  $k$ -dependence. Potential scattering of arbitrary strength  $1-w$  is included.  $H_{\text{int}}$  represents the e-e interaction:

$$H_{\text{int}} = \frac{g}{\pi} \int_0^\infty dk_1 \dots \int_0^\infty dk_4 \sum_{\alpha, \beta, \gamma = \pm} \delta(k_1 + \alpha k_2 + \beta k_3 + \gamma k_4) c_{k_1 a}^\dagger c_{k_2 b}^\dagger c_{k_3 b} c_{k_4 a}. \quad (2)$$

In listing some of the properties of the model (1) let us start by listing the pleasing aspects.

(i) The eigenstates of (1) are Bethe wavefunctions, and so the corresponding exact energy eigenvalues can be found.

(ii) Deleting the second term in (1) leads to the Hamiltonian  $H_b$  of the pure host (index b for bulk).  $H_b$  can be diagonalised exactly, too. Due to this, impurity effects can be obtained by subtraction.

(iii) Obviously, the bare spectrum of (1) is bounded from below. There are thus no cut-off problems (see the introduction of I).

(iv) For repulsive e-e interaction there are no pathologies in the behaviour of the band electrons. Note, that (as the model is effectively one-dimensional) attractive interaction would lead to bound pairs of electrons (see also the conclusions of I).

We now go on to rather unfortunate properties.

(v) Only electrons in s-wave states are included in (1). This means that there is no interaction of s- with p-waves etc.. All bulk properties noticed (as e.g. those in (ii) and (iv)) refer to the s-wave subsystem.

(vi) The same coupling  $g$  governs the e-e interaction (2) and the impurity term. This relation is dictated by solvability.

(vii) The matrix element in (2) has a rather special form (again dictated by solvability), which refers to a non-local two particle interaction (see also I and Appendix 1 therein). Equation (2) means that, in preparing the s-wave subsystem, only a few special types of transitions are retained. Nevertheless, these are repulsive.

All the work on the stationary Schrödinger equation with Hamiltonian (1) may be grouped in two halves. The first half ends with the formal solution—see (7) and (8) below—i.e. with non-linear algebraic equations for the quasi-momenta which determine the energy eigenvalues. Then, in the second half the physics has to be worked out ('real solution'). As the analysis in the first half does not depend on the sign of the coupling, it is completely contained in I. Hence the present paper is restricted to the analysis required in the second half, and we may start from the formal solution. Nevertheless, let us briefly remember the main steps that lead from (1) to (7) and (8).

By changing the meaning of the creation operators  $c^\dagger$  (let  $c_{ka}^\dagger$  create a  $\cos(kx)$  state) the problem (1) is placed on a fictitious  $x$  axis with states of even parity only (see I). In 'first quantisation' and in the  $N$ -particle sector the new Hamiltonian reads

$$H = \sum_{j=1}^N (-\partial_{x_j}^2) - 2g \sum_{j=1}^N \delta(x_j) (\tau \sigma_j + 1 - w) + 4g \sum_{i < j}^N [\delta(x_i - x_j) + \delta(x_i + x_j)] . \quad (3)$$

(3) has the same spectrum as (1), and the s-wave many-body eigenstates of (1) are related to those of (3) by a unitary transformation (stated explicitly in I). On omitting the second sum, equation (3) turns into the bulk Hamiltonian. In both problems the number of down spins  $M$  is conserved. Due to this, the model is easily extended to include an applied magnetic field:

$$H \longrightarrow H - \mu_0 B \sum_{j=1}^N \sigma_j^z - \mu_0 B \tau^z \longrightarrow E(N, M) - (N + 1 - 2M) \mu_0 B . \quad (4)$$

The Bethe wavefunctions are made up of  $\exp(ikx)$  factors (see I), refer to spatial ranges separated by the delta interactions in (3), and are to be complemented by passage formulas connecting these ranges. Factorisation can be shown. Let the  $x$  axis be bound to a circle of circumference  $2L$ . The corresponding periodic boundary conditions lead to  $N$  equations for  $N$  quasi-momenta  $k_j$  depending on the solution of a further matrix-eigenvalue problem in the spin degrees of freedom. Its treatment (Schulz 1985) by a second Bethe *ansatz* leads to  $M$  equations for  $M$  spin momenta  $\vartheta_r$ . These  $N + M$  coupled equations (see (44) in I) constitute the formal solution, whereas the energy is simply the sum of the  $N$  squared  $k$ -momenta. For convenience we introduce dimensionless energy, coupling and momenta via

$$E = g^2 \varepsilon \quad g = v/L \quad k_j = g q_j \quad \gamma_r = g \vartheta_r . \quad (5)$$

Note that  $v$  may be interpreted in two ways, as an effective coupling ( $v \rightarrow 0$  for  $g \rightarrow 0$  at fixed  $L$ ) and as an effective length that diverges in the thermodynamic limit ( $v \rightarrow \infty$  for  $L \rightarrow \infty$  at fixed  $g$ ). Turning on the interaction, the  $k$ -momenta start off as multiples of  $\pi/L$  while the new momenta ( $q = k/g = \text{multiples of } \pi/v$ ) start at plus infinity and decrease.

With (5), the formal solution to the energy eigenvalues of (1) reads as follows:

$$\varepsilon = \sum_{j=1}^N q_j^2 \quad (6)$$

$$\exp(-i2vq_j) = \left[ \frac{q_j + i(2-w)}{q_j - i(2-w)} \right] \prod_{r=1}^M \frac{q_j + \gamma_r - i}{q_j + \gamma_r + i} \frac{q_j - \gamma_r - i}{q_j - \gamma_r + i} \quad (j = 1, \dots, N) \quad (7)$$

$$\begin{aligned} & \left[ \frac{\gamma_r + i(1-w)}{\gamma_r - i(1-w)} \frac{\gamma_r + i(1+w)}{\gamma_r - i(1+w)} \right] \prod_{j=1}^N \frac{\gamma_r + q_j + i}{\gamma_r + q_j - i} \frac{\gamma_r - q_j + i}{\gamma_r - q_j - i} \\ & = \prod_{s=1}^M \frac{\gamma_r + \gamma_s + 2i}{\gamma_r + \gamma_s - 2i} \frac{\gamma_r - \gamma_s + 2i}{\gamma_r - \gamma_s - 2i} \quad (r = 1, \dots, M) . \end{aligned} \quad (8)$$

If the factors in square brackets are omitted, equations (7) and (8) refer to the bulk system (no impurity). Equations (7) and (8) are almost identical (apart from some signs) to the equations (47) and (48) of I. This small difference, however, leads to a quite different ground state structure, to different integral equations and to different physics. So things have to be done anew (Göhmann 1989). However, the analysis in I is used for orientation†.

In section 2 we find the structure of the ground state at a given down-spin number  $M$ . In section 3 integral equations are derived that determine the excess impurity energy in the thermodynamic limit. In section 4 the impurity magnetisation is defined, related to more suitable integral equations and evaluated at low applied magnetic field. The resulting impurity susceptibility is singular and non-perturbative. In contrast, as is shown in section 5, the bulk behaves rather normally. A Stoner factor is derived. It is, however, smaller than that resulting from perturbation expansion.

## 2. The lowest energy at given $M$

In order to calculate the magnetisation at a given applied field  $B$  in the thermodynamic limit, we need to know the lowest energy in the  $N, M$ th sector of the Hilbert space as a smooth function of  $M$ . The system minimises the expression (4), where  $E$  is this function. If we do so as well, the desired  $M, B$  relation will arise.

All the information required is contained in (6) to (8). An eigenstate of  $H$  corresponds to a set of  $q$ -values that solves (7) and (8). We do not know, however, whether each solution of (7) and (8) gives a physically admitted state or not‡. The way out of this predicament is by reading (7) and (8) as 'equations of motion' to be supplied with initial values at 'time' zero:  $v = 0$ . At zero coupling the eigenstates of  $H$  (and of  $H_b$ ) are Fock states. They certainly form a complete basis for the Hilbert space. The Fock state of lowest energy in sector  $N, M$  is doubly occupied at the lowest  $M$  positions  $j\pi/L$  ( $j = 0, 1 \dots$ ) followed by  $N - 2M$  singly occupied positions. The initial condition for the impurity spin is 'up', if  $B > 0$  (as we shall always assume). We also know the  $M$  initial values of the  $\gamma$  set. They agree with the first  $M$   $k$ -values, since the only possible way for two  $k$ -values to become equal for  $v \rightarrow 0$  is to form a 'sandwich' with one  $\gamma$ -value in between (Schulz 1985).

With these initial values in mind, changing to the dimensionless language (5) and using (7) and (8) at small coupling, we obtain the asymptotically leading terms ( $v \rightarrow 0_+$ ) of all momenta

$$q_1 = iv^{-1/2}((5 + 2w)^{1/2} - 1 - w)^{1/2} \quad (9a)$$

$$q_2 = v^{-1/2}((5 + 2w)^{1/2} + 1 + w)^{1/2} \quad (9b)$$

$$\gamma_1 = v^{-1/2}(2 + w)^{1/2} \quad (9c)$$

$$q_{2j} = q_{2j-1} = v^{-1}(j - 1)\pi \quad (j = 2, \dots, M) \quad (9d)$$

† A few errors in I (in addition to those noticed in a corrigendum) might be corrected as follows: (47): the sum is a product; (61): take the first sum twice; (62): the fourth sign is  $-$ ; below (85):  $v = v(a)$ ; second line of (88): the second sign is  $+$ ; below (95):  $n, m \rightarrow \infty$ , i.e.  $a, c \rightarrow \infty$ ; (103): the second kernel is  $K$ ; (117): the second sign is  $+$ ; (129): the first term in the numerator is  $e$ .

‡ For example, the Bethe wavefunction could vanish. This is the case for  $\gamma_1 = 0$ , which trivially solves the first equation (8). Furthermore, overcounting has to be avoided by suitable restrictions (see I). But, even apart from these examples, there could be less trivial unphysical solutions of (7) and (8).

$$q_j = v^{-1}(j - M - 1)\pi \quad (j = 2M + 1, \dots, N) \quad (9e)$$

$$\gamma_r = v^{-1}(r - 1)\pi \quad (r = 2, \dots, M). \quad (9f)$$

For the bulk case (no impurity), equations (9a)–(9c) are to be replaced by  $q_1 = 0$  (remaining zero for all  $v$ ),  $q_2 = 2v^{-1/2}$ ,  $\gamma_1 = (v/2)^{-1/2}$ . As (9a) shows, one electron of the lowest sandwich has become bound to the impurity. This bound state persists up to  $w = 2$  (replace  $\sigma\tau + 1 - w$  in (3) by  $2 - w$  for parallel spins). The potential scattering becomes attractive below  $w = 1$ , and below  $w = -2$  a second electron is bound to the impurity. We shall keep away from this value (for formal reasons) and restrict ourselves to the range

$$-1 < w < 2 \quad (10)$$

which is qualitatively uniform. The singular behaviour of the impurity susceptibility does not depend on the presence of a bound state. It is even independent of  $w$  (see section 4).

In the course of increasing ‘time’  $v$ , the momenta leave their special initial values (9a)–(9f), but the structure of their positions in the complex plane is always maintained: one  $q$  purely imaginary and the others real. We state this as an assumption, which will be verified below. Consider, for example, (7) for  $j = 1$  and write  $q_1 = ip$ :

$$\exp(2vp) = \frac{p + (2 - w)}{p - (2 - w)} \prod_{r=1}^M \frac{\gamma_r^2 + (p - 1)^2}{\gamma_r^2 + (p + 1)^2}. \quad (11)$$

From (11) it is obvious, that  $p$  remains real, decreases and ends up at  $2 - w$  when  $v \rightarrow \infty$ , where the difference from this value becomes exponentially small. In the remaining equations (7) and (8) (even after inserting  $q_1 = ip$ ) there are only phase factors. If one carefully watches the ‘time’ development of each phase (see I for details), taking logarithms is a unique procedure. The resulting equations are

$$\varepsilon = [-p^2] + \sum_{j=2}^N q_j^2 \quad (12)$$

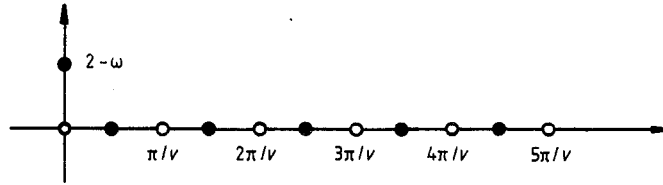
$$vq_j = (j - 1)\pi + \left[ a\left(\frac{q_j}{2 - w}\right) - \frac{\pi}{2} \right] - \sum_{b=\pm} \sum_{r=1}^M a(q_j + b\gamma_r) \quad (j = 2, \dots, N) \quad (13)$$

$$2a(\gamma_r) + \sum_{b=\pm} \sum_{j=2}^N a(\gamma_r + bq_j) = r\pi + [A(\gamma_r, p)] + \sum_{b=\pm} \sum_{s=1}^M a\left(\frac{\gamma_r + b\gamma_s}{2}\right) \quad (r = 1, \dots, M) \quad (14)$$

with  $a(x) \equiv \tan^{-1}(x)$  and

$$A(\gamma, p) \equiv a\left(\frac{1 - w}{\gamma}\right) + a\left(\frac{1 - p}{\gamma}\right) + a\left(\frac{1 + w}{\gamma}\right) + a\left(\frac{1 + p}{\gamma}\right) - 2a\left(\frac{1}{\gamma}\right). \quad (15)$$

Here,  $p$  is  $-iq_1$ , and the prime excludes  $s = r$ . The bulk equations are obtained by omitting all the terms in square brackets in (12)–(14). Equations (11) to (15)



**Figure 1.** Positions of the quasi-momenta in the complex plane for infinitely strong coupling: full circles refer to the system with impurity and the open circles refer to the system without impurity.

contain all information on the exact lowest energy for *finite* numbers  $N, M$  (as long as  $2M < N + [1]$ ). The expressions allow for  $g \rightarrow 0$  (i.e., they are ‘perturbative’). The reader can readily check them for  $N = 1, 2$  and they lead to the  $q$ -positions of figure 1 in the limit of infinite coupling  $g \rightarrow \infty$  ( $L, M, N$  finite), since then all  $a$ -functions in (13) can be neglected.

From (13) and (14) it can be shown (Göhmann 1989) that two  $q$ -values (or two  $\gamma$ -values) can never become equal at a finite coupling  $v$ , and that  $\gamma_1$  never reaches zero. This justifies our initial assumption of an unchanged structure of positions (see figure 1) for all couplings  $v$ .

These statements refer to that unique state in the  $N, M$  sector that has lowest energy at (or near to) ‘start time’,  $v = 0$ . No other state in this sector may develop a lower energy at higher  $v$ . Arguments in support of this conjecture are given in I.

### 3. The thermodynamic limit

As is well known, the discrete equations (11) to (15) turn into tractable integral equations in the thermodynamic limit  $N, M, v \rightarrow \infty$  at fixed  $g$  and fixed ratios

$$n = \frac{N}{gL} = \frac{N}{v} \quad m = \frac{N - 2M}{gL} = \frac{N - 2M}{v} \tag{16}$$

They determine the leading, i.e. the extensive, term in the energy  $\varepsilon$ . The excess energy due to the impurity

$$\varepsilon - \varepsilon_b = -U \tag{17}$$

is, however, an intensive quantity. The subscript b refers to the bulk version of (13) to (15). We expect a negative excess ( $U$  positive), since additional degrees of freedom might allow for a lower energy in the  $M-N$  sector. The appropriate procedure for treating an intensive difference effect is due to Gaudin (1971): derive (still discrete) equations for difference momenta by subtracting the corresponding bulk equations; restrict yourself to the intensive terms; perform the ‘partial limit’ ( $p \rightarrow 2 - w$  in our case here) for quantities saturating exponentially; consider the difference momenta to form a function of the ordinary momenta and relate it to their density; extend to negative values as an odd function for convenience. Following this recipe with the initial ingredients being (13) to (15), we define the bulk densities

$$\rho(q) = \frac{d(j\pi/v)}{d(2\pi q)} \quad \sigma(\gamma) = \frac{d(r\pi/v)}{d(2\pi\gamma)} \tag{18}$$

as even functions of their arguments, write  $\kappa(q)$  to represent the function that the  $q$ -differences turn into (and  $\eta(\gamma)$  for the  $\gamma$ -differences) and introduce

$$f(q) = 4v\rho(q)\kappa(q) \quad h(\gamma) = 4v\sigma(\gamma)\eta(\gamma) \tag{19}$$

as odd functions of  $q$  or  $\gamma$ , respectively. Since the procedure and notation are similar to those in I, we might emphasise that here the densities  $\rho$ ,  $\sigma$ ,  $f$  and  $h$  occur with a different physical meaning.

For the excess energy (17)

$$U = (2 - w)^2 - \frac{1}{2} \int_{-d}^d dx x f(x) \tag{20}$$

the following integral equations arise:

$$f = \xi + \int_c D_1 h \quad h = \phi + \int_d D_1 f - \int_c D_2 h \tag{21}$$

with

$$\xi = -\frac{2}{\pi} a \left( \frac{2 - w}{x} \right) \tag{22}$$

$$\phi = \frac{2}{\pi} \left[ a \left( \frac{3 - w}{x} \right) + a \left( \frac{1 + w}{x} \right) - 2a \left( \frac{1}{x} \right) \right].$$

In (21) all the terms are functions of  $x$ . The shorthand notation used for integrals becomes obvious from

$$\int_c^d D_2 h = \int_{-c}^c dy D_2(x - y)h(y) \quad D_n(x) = \frac{1}{\pi} \frac{n}{n^2 + x^2} \quad (n = 1, 2). \tag{23}$$

Clearly, (21) and (22) determine  $U$ , equation (20), if the integration limits  $c$  and  $d$  are known. These are to be obtained from the bulk information

$$\int_{-d}^d dx \rho(x) = n \quad \int_{-c}^c dx \sigma(x) = \frac{n - m}{2} \tag{24}$$

where the bulk densities derive from

$$\rho = \frac{1}{2\pi} + \int_c D_1 \sigma \quad \sigma = \int_d D_1 \rho - \int_c D_2 \sigma. \tag{25}$$

With the solution  $\rho$  of (25) one also obtains the bulk energy density

$$V = \frac{\epsilon_b}{v} = \int_{-d}^d dx x^2 \rho(x). \tag{26}$$

The only input that activates the machinery of (20) to (25) consists of the two real variables  $m$  and  $n$ . The excess and bulk energies, (20) and (26), are thus functions of only these two:  $U(n, m)$ ,  $V(n, m)$ .



The integral equations (25) are identical to those of Yang (1967) for the delta-interacting one-dimensional Fermi gas (cf also Takahashi (1970) and Schulz (1985)). In order to understand the effects of the impurity we need to understand some characteristics of the bulk. To begin, let us turn off the interaction and calculate the Pauli susceptibility  $\chi_0$ . Since for  $g \rightarrow 0$  we have  $n, m \rightarrow \infty$  and  $c, d \rightarrow \infty$ , the kernels  $D$  in (25) act like delta-functions. The solution of (25) is then easily obtained as

$$\rho = (1 + \Theta_c \Theta_d)/2\pi \quad \sigma = \Theta_d/2\pi \tag{27}$$

with  $\Theta$  a step function (equal to one inside  $(-c, c)$  or  $(-d, d)$  and zero otherwise). Equations (16), (26), (27) and the condition  $c < d$  lead to

$$\begin{aligned} V &= (n^3 + 3nm^2)\pi^2/12 & \dot{V} &= nm\pi^2/2 & (\text{dot} \equiv \partial_m) \\ (N - 2M)/2L &\equiv \chi_0\mu_0B & \chi_0 &= L/\pi^2N = z_f & (g = 0) \end{aligned} \tag{28}$$

where  $z_f$  is the density of states (per length  $2L$ ) of our special s-wave system. To derive the second line in (28) we used the general  $B, M$  relation

$$b = \dot{V}(n, m) \quad (\mu_0B/g^2 \equiv b) \tag{29}$$

which is obtained by minimising (4), with (5) and (26) used for  $E$ .

Next we study the large- $x$  asymptotics of (25) for  $g > 0$ ,  $\rho \simeq 1/2\pi$ ,  $\sigma \simeq m/\pi x^2$ , and note that we are allowed to integrate the second relation (25) over all  $x$ . This leads to

$$\int_c dx \sigma(x) = m \quad \left( \int_c \equiv \int_{-\infty}^{-c} + \int_c^{\infty} \right) \tag{30}$$

and shows that zero magnetisation  $m \rightarrow 0$  corresponds to  $c \rightarrow \infty$ . Remember that  $c < d$  holds for the non-interacting system. Thus, we observe an extremely different behaviour of the interacting system. The two limits  $g \rightarrow 0$  and  $N - 2M \rightarrow 0$  do not commute. This is intimately related to the system's singular property to be detailed in the remainder.

We turn now to considering the change of  $c$  (and of  $d$ ) with increasing magnetisation  $m$ . By differentiating (24) with respect to  $m$  we get

$$2\dot{d}\rho(d) = - \int_d \dot{\rho} = -u(d)/2 \quad 2\dot{c}\sigma(c) = - \int_c (\frac{1}{2}\delta(x) + \dot{\sigma}) = -v(c)/2 \tag{31}$$

where on the right hand side of each equation in (31) a new odd function has been defined via  $4\dot{\rho}(x) \equiv \partial_x u(x)$  and  $2\dot{\delta}(x) + 4\dot{\sigma} \equiv \partial_x v(x)$ , respectively. Integral equations for this new pair of functions are derived from (25)

$$u = \varphi_u + \int_c D_1 v \quad v = \varphi_v + \int_d D_1 u - \int_c D_2 v \tag{32}$$

with

$$\varphi_u = -\frac{2}{\pi}a(x) \quad \varphi_v = \text{sgn}(x) + \frac{2}{\pi}a\left(\frac{x}{2}\right) . \tag{33}$$

Note that by now all pairs of integral equations have the same form. To solve (32) for large  $c$ , we first rewrite them as

$$u = \varphi_u + \int D_1 v - \int D_1 \bar{v} \quad v = \varphi_v + \int D_1 \bar{u} - \int D_2 v + \int D_2 \bar{v} \tag{34}$$

with  $\bar{u} \equiv u \Theta_d$  and  $\bar{v} \equiv v(1 - \Theta_c)$ . Then we carry out a Fourier transformation and solve for  $u, v$  (as if  $\bar{u}, \bar{v}$  were known functions). This leads to

$$u = \psi_u + \int_d R u - \int_c K v \quad v = \psi_v + \int_d K u + \int_c R v \quad (35)$$

with

$$\psi_u = \varphi_u + \int K \varphi_v = 0 \quad \psi_v = \varphi_v - \int R \varphi_v = \text{sgn}(x). \quad (36)$$

The kernel  $R$  is defined by its Fourier transform  $1/(\exp(2|k|)+1)$ ,  $K(x) = 1/4 \cosh(x\pi/2)$ . Examining (35) at large  $c$ , we use the properties

$$\int dx K(x) = \int dx R(x) = \frac{1}{2} \quad R \simeq \frac{1}{2\pi x^2} \quad K \simeq \frac{1}{2} \exp(-\pi x/2) \quad (x \rightarrow \infty) \quad (37)$$

and notice that  $u(d)$  is exponentially small, while  $1 < v(c) < 2$ . For the remaining two quantities in (31) we know  $1/2\pi < \rho(d) < 1/\pi$ , while  $\sigma(c)$  is exponentially small. To see this, transform (25) into

$$\rho = \frac{1}{2\pi} + \int_d R \rho - \int_c K \sigma \quad \sigma = \int_d K \rho + \int_c R \sigma \quad (38)$$

and use (37) again.

To summarise:

$$\dot{d} = -\frac{u(d)}{4\rho(d)} = O(\exp(-\pi c/2)) \quad \dot{c} = -\frac{v(c)}{4\sigma(c)} = -\lambda \exp(\pi c/2) \quad \lambda = O(1). \quad (39)$$

Turning on the magnetic field or, equivalently, increasing the bulk magnetisation  $m$ , leads to an unimportant change of the integration limit  $d$ . However,  $c$  decreases rapidly. We have now collected the bulk information that we need in the next section to study the impurity effects.

#### 4. Impurity magnetisation

When the impurity is introduced into the host metal, there is, on the one hand, the change  $U(n, m)$  of energy (see (20) to (22)), and, on the other hand, a change  $\Delta$  of the integrated magnetisation:  $m \rightarrow m + \Delta$ . The two changes become related through energy minimisation:

$$\partial_\Delta [vV(n, m + \Delta) - U(n, m + \Delta) - b - (m + \Delta)vb] = 0. \quad (40)$$

The intensive quantities in (40) are  $V, U, m, b$  and  $v\Delta$ . Using (29) and restricting ourselves to the leading (namely intensive) terms of (40), we obtain  $v\Delta = \dot{U}/\dot{V}$ . If the impurity magnetisation  $\mu$  is defined as the increase in up-minus-down numbers, we have  $\mu = 1 + v\Delta$  and thus

$$\mu(n, m) = 1 + \dot{U}/\dot{V} \quad (41)$$

To treat (41), the derivatives (dots) with respect to  $m$  have to be made explicit. This is possible in general (Göhmann 1989). Here we seek for a shorter, more transparent way that works in the limit of small  $m$  (i.e. small  $B$  and large  $c$ ). We start by differentiating (26) with respect to  $m$ :

$$\dot{V} = -\frac{1}{2} \int_{-d}^d dx xu(x). \tag{42}$$

Equation (42) still holds true exactly and is remarkably similar to (20) for  $U$ , except for the additional constant in (20). This constant disappears on a further dot-differentiation as required by (41). At this point we exploit (39) and neglect terms  $O(\exp(-\pi c/2))$  (such as  $\dot{d}$ , but so far no powers of  $c$ ):

$$\dot{U} = -\frac{1}{2} \int_{-d}^d dx x\dot{f} \quad \dot{V} = -\frac{1}{2} \int_{-d}^d dx x\dot{u}. \tag{43}$$

Consider now the integral equations (21) and (32) for  $f$  and  $u$ , respectively. The different inhomogeneities disappear under the dot-operation, and the resulting integral equations for  $\dot{f}$  and  $\dot{u}$  are identical (neglecting  $\dot{d}$ ), except for constant prefactors in the (new) inhomogeneities. We conclude that

$$\dot{f}(x)/h(c) = \dot{u}(x)/v(c) \tag{44}$$

and consequently

$$\mu = 1 + h(c)/v(c). \tag{45}$$

We are left with equation (21) for  $h$  (and (32) for  $v$ ). It is here that the impurity details (22) appear. For large  $x$  (namely  $x$  of order  $c$  in magnitude) we may neglect the  $f$ -term in the second equation (21). It is of order  $\exp(-\pi c/2)$  (Göhmann 1989). We may also use the asymptotics  $\phi(x) \simeq 4/\pi x$  of (22). It may even be replaced by the constant  $4/\pi c$ . This rather intuitive step can be justified in detail. Hence, if we restrict ourselves to the leading power in  $c$ , we may write

$$h(x) = \frac{4}{\pi c} - \int_c^x D_2 h \quad v(x) = 2 - \int_c^x D_2 v \tag{46}$$

and read off that  $h(x) = 2v(x)/\pi c$  for large  $x$ . This way we are led to

$$\mu = 1 + \frac{2}{\pi c} + O\left(\frac{\ln(c)}{c^2}\right) \tag{47}$$

where the O-term is added by conjecture (based on iteration).

Equation (47) is our main result. On turning off the magnetic field ( $c \rightarrow \infty$ ) there remains no net magnetic moment, except for the half-spin itself ( $\mu \rightarrow 1$ ). This might be due to point (v) of the introduction, i.e. to the one-dimensionality of the model. To study the slope of the  $\mu$  over  $B$  curve, given by (47) rather implicitly, we calculate the susceptibility. By analogy with (28) we define it by

$$\chi = \partial_{\mu_B}(N - 2M)/2L = (\partial_b m + \partial_b \mu/v)/2g \equiv \chi_b + \chi_{\text{imp}} \tag{48}$$

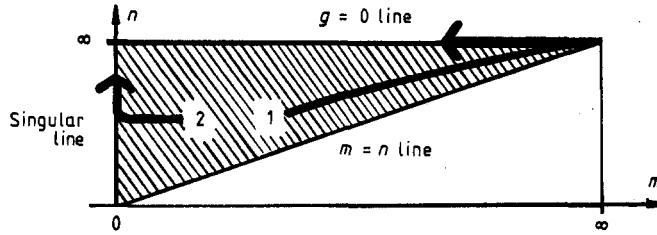


Figure 2. Range in the  $nm$  plane, over which all system-specific functions are defined.

where so far only the definitions of  $m, b, \mu$  have been used (see (16) and the text above (41)). For the bulk susceptibility, (29) tells us that

$$\chi_b(n, m) = \frac{1}{2g\dot{V}(n, m)} \quad (49)$$

and for the impurity part, (47) and (39) give

$$\chi_{\text{imp}} = \chi_b \mu / v = \chi_b \lambda \exp(\pi c / 2) (2 / \pi c^2 v). \quad (50)$$

For  $\lambda$  see (56) and (57) below. To eliminate  $c$  in favour of  $m$ , we consider (39) as a differential equation and solve for  $c$ :

$$\lambda \exp(\pi c / 2) = 2 / \pi m \quad c = (2 / \pi) \ln(1 / m) + O(1). \quad (51)$$

By means of (51) and (16) the impurity magnetisation is re-expressed in terms of the original parameters:

$$\chi_{\text{imp}} = \chi_b \frac{1}{(N - 2M)} \left[ \ln \left( \frac{Lg}{N - 2M} \right) \right]^{-2}. \quad (52)$$

Now the expected non-perturbative nature of the susceptibility is obvious. Equation (52) should be compared with the susceptibility of the relativistic Kondo model. For spin- $\frac{1}{2}$  and high field this susceptibility agrees with (52) (Wiegmann (1981): equation (73); Andrei *et al* (1983): equation (4.33)). For higher spin, however, even the low-field susceptibility agrees with (52) (Andrei *et al* (1983): equation (7.3)). Remember that, for our model and for  $g > 0$ , there is no Kondo regime (the half spin is not screened).

Inverse logarithms are also encountered in nearby systems. For the ferromagnetic spin- $\frac{1}{2}$  Heisenberg chain at low temperature (Schlottmann 1986)  $\partial_T(T\xi)$  behaves as (52) with  $T$  replacing  $N - 2M$  and  $\xi$  the correlation length. The same is true for  $\partial_T(T^2\chi)$  with  $\chi$  the susceptibility of a spin- $S$  impurity ( $S > 1$ ) imbedded in a spin-1 Heisenberg chain (Lee and Schlottmann 1988).

Apart from the singular initial increase of the impurity magnetisation, there is no further pronounced behaviour at higher fields. Most probably the impurity magnetisation increases monotonically and reaches the maximum value at  $m \rightarrow n$ , i.e. at vanishing down spin number, i.e. along the diagonal border line in figure 2. The value along this line (Göhmman 1989) is given by

$$\mu = 1 + a \left( \frac{2 - w}{\pi n} \right) \frac{1}{a(\pi n)}. \quad (53)$$

It can also be shown that  $\mu$  decreases when deviating from this line.

5. Stoner factor

For the physical interpretation of the impurity effect in the preceding section it was understood that the bulk system behaves normally. In particular, the bulk susceptibility might have a finite value at zero field. Exchange enhancement of this value is presumed such that the Pauli susceptibility (28) comes out in the limit of zero coupling, and a Stoner factor arises to first order. This section is devoted to proving or disproving these conjectures.

There are several reasons for doubting fully normal bulk behaviour. We are warned, for example, by the highly unusual bulk properties observed in I, i.e. in the Kondo case of the present model. A more direct warning is inherent in a result of Takahashi (1970) on the ground state energy  $V$ , (26). Note that the bulk is described by the Yang equations. According to Takahashi's 'conjecture 1',  $V$  is singular at the point  $g = 0$  and  $m = 0$ , which is the upper left corner of the  $nm$  plane in figure 2. Certainly, this property (if true) is related to the non-commutativity of limits as noticed below (30). These two limits correspond to qualitatively quite different paths through the  $nm$  plane, see figure 2. The term 'different', of course, depends on the quantity studied. The zero-field susceptibility, to start with, was obtained along path 1 in section 3. Here we follow path 2, to see whether it also results in the Pauli susceptibility (28).

We start with (49) and take the limit  $m \rightarrow 0$  first. To calculate  $\ddot{V}(n, 0)$  from (43), the pair of integral equations for  $\dot{u}$  and  $\dot{v}$  has to be studied in the limit  $c \rightarrow \infty$ . By deriving this pair via dot-differentiation of (35), using (39), exploiting the kernel properties (37), introducing the function  $r(x) = v(x + c)$  and using the integral equation for  $r'(x)$ , we obtain

$$\ddot{V}(n, 0) = C\lambda(d)F(d)\pi/4 \quad C = \int_0^\infty dx \exp(-\pi x/2)r(x) \quad F(d) = \int_{-d}^d dx xt(x). \tag{54}$$

The functions  $r$  and  $t$  are defined as the solutions of

$$r(x) = 1 + \int_0^\infty Rr \quad t(x) = \sinh(\pi x/2) + \int_d R t \tag{55}$$

and

$$\lambda(d) = \lim_{c \rightarrow \infty} r(0) \exp(-\pi c/2)/4\sigma(c) \tag{56}$$

is just the constant  $\lambda$  that was introduced in (38). To evaluate it, we use (38) with (37) and obtain

$$\lim_{c \rightarrow \infty} \sigma(c) \exp(c\pi/2) = r(0)/4\lambda(d) = s(0)G(d)/2 \quad G(d) = \int_{-d}^d dx \cosh(\pi x/2)\rho(x) \tag{57}$$

where  $s$  and  $\rho$  are defined as the solutions of

$$s(x) = 1 + \int_0^\infty dy R(x-y) \exp[(x-y)\pi/2]s(y) \quad \rho(x) = \frac{1}{2\pi} + \int_d R\rho. \tag{58}$$

Equations (55) and (58) imply the identity

$$s(0)r'(x) = r(0)s'(x) \exp(-\pi x/2). \tag{59}$$

Combining the results (57) and (54) with (49) we obtain the exact zero-field susceptibility of the interacting host metal as

$$\chi_b(n, 0) = \frac{4}{\pi g} \frac{1}{C} \frac{s(0)}{r(0)} \frac{G(d)}{F(d)}. \tag{60}$$

It depends on the particle density  $n$  through  $d$  and (24).

Could it happen that, as  $g \rightarrow 0$ , this rather involved expression (60) turns into the simple Pauli susceptibility (28)? It does indeed, as we now show.  $g \rightarrow 0$  means  $d \rightarrow \infty$  and corresponds to the vertical part of path 2 in figure 2. Consider  $G(d)$  first. If we restrict ourselves to the leading terms ( $d$  large), we may replace  $2\pi\rho(d-x)$  by  $r(x)$  (compare their integral equations with each other). This leads to

$$G(d) = \exp(\pi d/2) C/2\pi \quad \check{V}(n, 0) = \pi^2 r(0) \exp(-\pi d/2) F(d)/4s(0). \tag{61}$$

By treating  $F(d)$  in a similar manner (where  $t(x)$  may be replaced by  $s(d-x) \exp(x\pi/2)$ ), and by using (59), we obtain

$$\check{V}(n, 0) = -r(2d)d\pi/2 + \int_0^{2d} dx r(x)\pi/2 = \pi d + O(1) \tag{62}$$

where the second equality arises from  $r(\infty) = 2$ , which is obvious from (55) and (37). Since, by (24),  $d \rightarrow n\pi/2$ , we see that the Pauli susceptibility (28) results.

At large coupling  $g$  ( $d$  small) the bulk susceptibility (60) increases as  $1/d^2$ . We may thus state (without proof) that it is a monotonically decreasing function of  $n$  (upward along the vertical axis in figure 2). It is then tempting to search for a Stoner factor at small but non-zero coupling  $g$  ( $n$  and  $d$  large). This requires including the next order terms in (62). A somewhat lengthy analysis leads to

$$G(d) = \exp(\pi d/2) (C/2\pi) (1 - 1/2\pi d) \tag{63}$$

$$F(d) = \exp(\pi d/2) (2/\pi) (s(0)/r(0)) \left( \int_0^{2d} dx r(x) - 2d - 3/\pi \right)$$

to be complemented by the  $n$ - $d$  relation

$$\pi n = -2d + \int_0^{2d} dx r(x) + O(1/d). \tag{64}$$

Through (60), (63) and (64) the bulk susceptibility is obtained as

$$\chi_b(n, 0) = \frac{\chi_0}{1 - 2/n\pi^2} = \frac{\chi_0}{1 - 2gz_f/2L} \tag{65}$$

and includes the leading correction with respect to small coupling  $g$ . Equation (65) is a type of Stoner factor, but not the one obtained by perturbation expansion. To see this we follow path 1 in figure 2 and include  $g$ -terms to first order. Doing so, we use the zeroth-order result (27) under the integrals in (25), and evaluate and make use of (26) and (24). The result is  $\chi_0/(1 - 4/n\pi^2)$ . Thus perturbation expansion is misleading. It overestimates the correct exchange enhancement given by (65).

To sum up, the non-commutativity of limits still persists in the magnetic properties of the bulk. Fortunately, however, the leading term is insensitive to this singular behaviour. It remains finite and is independent of the order of limits. This is what we really need in order to understand the impurity result (52): the prefactor  $\chi_b$  is an unimportant constant.

## 6. Conclusion

The excess magnetisation of a spin- $\frac{1}{2}$  impurity placed in a paramagnetic host metal has been calculated. The host susceptibility is exchange enhanced itself. Thereby, the Bethe *ansatz* is shown to work well even for a local phenomenon *and* for a bare spectrum which is naturally bounded from below.

Imagine an advanced lecture on solid state theory which, after presenting standard many particle mechanisms on itinerant electrons, one likes to complement by giving an exact model calculation. If a translational invariant model is sufficient, the one-dimensional Hubbard model (or its continuous version: the 1D delta-interacting Fermi gas) would be the appropriate (and, in essence, only) candidate. If local phenomena are to be included, the 'relativistic' Kondo model is a poor candidate, since it needs additional hand-waving arguments to interpret the results physically ('cut-off after the solution'). The model worked through in this paper, however, is free of such artificial steps. The physics comes about rather straightforwardly and in accord with intuition.

There are many more questions one would like to answer regarding the magnetic impurity problem and even the model at hand. For example, the details of the spatial distribution of the local excess magnetisation so far remain unknown. Other open questions concern the effect of temperature and the properties of correlation functions. Still, it seems likely that for our model these problems can be solved.

## References

- Andrei N 1980 *Phys. Rev. Lett.* **45** 379–82  
Andrei N, Furuya K and Lowenstein J H 1983 *Rev. Mod. Phys.* **55** 331–402  
Gaudin M 1971 *Phys. Rev. A* **4** 386–94  
Göhmann F 1989 *Diplomarbeit* Universität Hannover  
Lee K and Schlottmann P 1988 *Phys. Rev. B* **37** 379–383  
Moriya T 1985 *Spin Fluctuations in Itinerant Electron Magnetism* (Berlin: Springer)  
— 1987 *Metallic Magnetism (Springer Topics in Current Physics 42)* ed H Capellman (Berlin: Springer)  
Schlottmann P 1986 *Phys. Rev. B* **33** 4880–6  
Schulz H 1985 *J. Phys. C: Solid State Phys.* **18** 581–601  
— 1987 *J. Phys. C: Solid State Phys.* **20** 2375–2403 (corrigendum 1987 **20** 4999)  
Takahashi M 1970 *Prog. Theor. Phys.* **44** 348–58  
Tsvetick A M and Wiegmann P B 1983 *Adv. Phys.* **32** 453–713  
Wiegmann P B 1980 *JETP Lett.* **31** 364–70  
— 1981 *J. Phys. C: Solid State Phys.* **14** 1463–78  
Yang C N 1967 *Phys. Rev. Lett.* **19** 1312–5