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Disordered magnetic impurities in uniaxial critical quantum spin chains

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Abstract. We calculate exactly the thermodynamics of ensembles of magnetic impurities with randomly distributed host–impurity couplings in the critical region of the uniaxial spin-1/2 quantum chain. We derive a finite set of integral equations describing the complete temperature and magnetic field dependence of the system. Exact numerical results for arbitrary values of temperature and external magnetic field are obtained. We show that for strong disorder the quenching of the impurity moments is absent. For weak disorder the screening persists, but with a critical non-Fermi-liquid behaviour of the magnetic susceptibility and specific heat. We point out that the 'easy-plane' magnetic anisotropy does not qualitatively change the behaviour of the thermodynamic characteristics of the disordered impurities in the antiferromagnetic chain. On the other hand, anisotropy of ferromagnetic type can enhance the tendency to quenching of the impurities for strong disorder.

1. Introduction

The study of the Kondo problem [1] which describes the effects of the exchange interaction between the spin of a magnetic impurity and the spins of itinerant electrons remains one of the most interesting problems of many-body physics. The Kondo effect is perhaps the best-known example in which modern theoretical methods like those of renormalization group (RG) theory, the Bethe *ansatz*, bosonization, and conformal field theory, have manifested their strength [2, 3]. The crossover from the strong-coupling to the weak-coupling regime is one of the most famous examples of non-perturbative effects in condensed matter theory.

In the last few years the interest in non-Fermi-liquid (NFL) behaviour of magnetic systems and metallic alloys has grown considerably. A large class of conducting non-magnetic materials do not behave as usual Fermi liquids (FL) at low temperatures. One of the best-known examples of such behaviour is the Kondo effect for multi- (n-) channel electron systems: for an impurity spin less than $n/2$, a NFL critical behaviour results [4]. The critical behaviour of a single magnetic impurity can also be connected with a quadrupolar Kondo effect or non-magnetic two-channel Kondo effect [4]. However, for most of the dirty metals and alloys in which the NFL behaviour was observed (see e.g. the recent reviews [5, 6] and references [7–10]), the magnetic susceptibility (χ) and low-temperature specific heat (c) usually manifest logarithmic or weak power-law behaviour with temperature (T). The resistivity linearly decreases with temperature showing a large residual resistivity. This is different from the predictions of the theory of the overscreened Kondo effect [3, 4].

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The last property together with the alloy nature of the compounds suggests that the disorder (a random distribution of localized f electrons or a random coupling to the conducting electron host) may play the main role in the low-temperature NFL character of such systems. The idea of (non-screened) local moments existing in disordered metallic systems has already been formulated, recently [11–13]. It was proposed that near the metal–insulator transitions (or for the sufficiently alloyed systems far from the quantum critical point), disordered correlated metals contain localized moments. The change in the interactions between the impurity sites and the host spins can be considered as a modification of the characteristic energy scale, the Kondo temperature T_K. At that scale the behaviour of the magnetic impurity manifests the crossover from the strong-coupling regime (for $T, h, \ll T_K, h$ being the magnetic field) to the weak-coupling regime $T_K \ll h, T$. The impurity spin behaves asymptotically freely in the weak-coupling case, and it is screened by the host spins in the strong-coupling case. The random distribution of the magnetic characteristics of the impurities (i.e. their Kondo temperatures) may be connected either with the randomness of exchange couplings of itinerant electrons with the local moments [12], or with the randomness of the densities of conduction electron states [11]. In fact, both types of randomness renormalize the single universal parameter—the Kondo temperature which characterizes the state of the magnetic impurity. In reference [8] the results of measurements of the magnetic susceptibility, NMR Knight shift, and low-temperature specific heat have been reported. To explain the observed features it was necessary to assume some disorder, with a Gaussian distribution of the Kondo temperatures. However, the model which was used for the explanation of the experiment was oversimplified [8]: the magnetization of a single magnetic moment was approximated by the Brillouin function $B(ah/T + bT_K)$, where a, b are constants. It was noted [8] that the data for the specific heat and Knight shift did not agree with those predicted by the simple theory, especially for non-zero values of the magnetic field. The disagreement could be caused either by an inadequate representation of the Kondo magnetization by the single-impurity theory, or by the simple replacement $T \to T + bT_K$ in the Brillouin function, or because of a not perfectly symmetric Gaussian distribution of the impurity couplings. The inhomogeneous magnetic susceptibility was confirmed very recently [14] by muon spin-rotation experiments. The role of the long-range (RKKY) coupling between the local moments was taken into account recently [15] (Griffiths phase theory) exhibiting properties qualitatively similar to those of models with non-interacting local moments [14]. In addition, the presence of the spin–orbit interaction in some disordered heavy-fermion alloys demands the study of magnetic anisotropy, which can play an essential role in the physics of disordered spin interactions [15].

It is known that the physics of a single magnetic impurity in a one-dimensional (1D) antiferromagnetic (AF) Heisenberg spin $S = \frac{1}{2}$ chain and that of a single Kondo impurity in a 3D free-electron host are described by similar Bethe *ansatz* theories [2, 18, 19], e.g. the magnetizations and the low-temperature magnetic specific heats of the impurity for the two models coincide. The spin-$\frac{1}{2}$ Heisenberg model is the seminal model for correlated many-body systems. Most of its static properties are exactly known. The spin-$\frac{1}{2}$ magnetic impurity manifests the total Kondo screening with the (marginal) FL-like low-temperature behaviour of the magnetic susceptibility and specific heat, i.e. finite values of $\chi(T)$ and $c(T)/T$ in the low-temperature limit [2, 4]. In other words, the moment of the impurity is quenched by the localized host spins and by the spins of the conduction electrons, respectively. The magnetic anisotropy of the Kondo exchange interaction between the impurity spin and the spins of the free-electron host was also taken into account exactly [2]. It was pointed out that the magnetic anisotropy does not change drastically the Kondo effect of a single impurity. On the other hand, for the integrable lattice models one can incorporate a finite concentration of

magnetic impurities [20] without destroying the exact solvability (this was impossible for the free-electron host [2], where only a single magnetic impurity can be embedded). Hence, for the random distribution of magnetic impurities we can suppose that low dimensionality is not essential for the Kondo screening. The absence of the magnetic ordering in the NFL Kondo systems [5] also confirms this assumption. Note also that recently a very thorough comparison of the experimental results for NFL behaviour of disordered heavy-fermion Kondo alloys was performed, obtaining very good agreement with theoretical predictions of the model for distributed Kondo temperatures [10]. It should be noticed though that the results were obtained in the framework of the single-magnetic-impurity Bethe *ansatz* solution [16], which cannot be applied to the multi-impurity case. However, we point out that our model reveals a behaviour of magnetic impurities in the spin-$\frac{1}{2}$ quantum chain very similar to that of a single impurity in the free-electron host. Hence our exact solution strongly supports the analysis and the conclusions as regards the effect of randomness of the distribution of Kondo temperatures for the magnetic impurities given in reference [10].

All this leads to the goal of our present investigation: to find exactly the thermodynamics of disordered ensembles of spin-$\frac{1}{2}$ magnetic impurities in the magnetically uniaxial spin-$\frac{1}{2}$ chain in the critical region, i.e. the domain of magnetic anisotropy where excitations of the homogeneous host are gapless. We will allow for various *random distributions of the impurity–host couplings* for *arbitrary* values of external magnetic field and temperature. The magnetic anisotropy parameter is assumed to be homogeneous for the host spins and for the impurity spins. The results for the non-zero-temperature behaviour for the best-known case of the (spin-isotropic) antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain have been announced in reference [17]. We point out that in our study we calculate *exactly* without any approximations the thermodynamic characteristics of a *disordered interacting* many-body system for various ranges of external magnetic fields, temperatures, and values of the longitudinal anisotropy ($\Delta = J^z/J^{x,y}$). In the 'easy-plane' regime with $|\Delta| < 1$, the system possesses an antiferromagnetic ground state for antiferromagnetic ($0 \leqslant \Delta \leqslant 1$) as well as ferromagnetic ($-1 < \Delta \leqslant 0$) anisotropies.

In this paper we will show that:

(i) for several kinds of strong disorder of the impurity–host couplings, the (Kondo) screening is absent;
(ii) for weaker disorder, the quenching persists, but with a NFL temperature behaviour of the magnetic characteristics;
(iii) in the antiferromagnetic chain the 'easy-plane' anisotropy does not drastically change the behaviour of the randomly distributed impurities; on the other hand, for the ferromagnetic case the increase of the anisotropy causes some increase of screening for models with strong disorder;
(iv) the magnetic field lifts the degeneracy and effectively enhances the quenching of the impurity spins, hence decreasing the effect of disorder.

We performed a comparison of our exact results with previous approximate ones and with experimental data on NFL alloys.

The paper is organized as follows. After the introduction in section 1, the method of the thermodynamic Bethe *ansatz* is introduced in section 2 for random ensembles of magnetic impurities in the 'easy-plane' spin-$\frac{1}{2}$ chain by use of the 'quantum transfer matrix' approach. In section 3 we present our results for the temperature and magnetic field dependence of the magnetic susceptibility and the specific heat obtained from numerical treatments of the non-linear integral equations. Section 4 contains a discussion and concluding remarks.

2. The Bethe *ansatz* approach and the 'quantum transfer matrix'

We investigate the thermodynamics of the spin-$\frac{1}{2}$ quantum chain with magnetic anisotropy of 'easy-plane' type ($|\Delta| \leqslant 1$) with spin-$\frac{1}{2}$ impurities. The Hamiltonian of the system has the form

$$H = \sum_j H_{j,j+1} + H_{imp}$$

where the host part is

$$H_{j,j+1} = \vec{S}_j \cdot \vec{S}_{j+1} + (\Delta - 1) S_j^z S_{j+1}^z$$

(the host exchange constant J ($=J^x = J^y$) is set to 2). We can parametrize the anisotropy, as usual, by $\Delta = \cos\gamma$. Here $\Delta = 1$ ($\gamma = 0$) corresponds to the isotropic antiferromagnetic Heisenberg model, whereas $\Delta = -1$ ($\gamma = \pi$) corresponds to the isotropic ferromagnetic Heisenberg model. The case $\Delta = 0$ ($\gamma = \pi/2$) is the well-known XY point, for which the Hamiltonian, by use of the Jordan–Wigner transformation, can be mapped onto the Hamiltonian of non-interacting spinless lattice fermions. The impurities' part of the Hamiltonian has some special form for exactly solvable lattice Hamiltonians. Suppose we have an impurity distribution, in which impurities are not nearest neighbours, then for the impurity situated between sites m and $m+1$ of the host we obtain [17, 19, 21]

$$H_{imp} = J_{imp}\big(\hat{B}_1(H_{m,imp} + H_{imp,m+1}) - H_{m,m+1} - \mathrm{i}B_2[H_{m,imp}, H_{imp,m+1}]\big) \tag{1}$$

where

$$J_{imp} = \sin^2\gamma/(\sinh^2\theta + \sin^2\gamma)$$

and $[\cdot,\cdot]$ denotes the commutator. The operator $\hat{B}_1$ modifies the Heisenberg-like interaction by multiplying the transverse terms with $\cosh\theta$, and $B_2 = \tanh\theta/\sin\gamma$ is a number. One can see that $\theta = 0$ corresponds to the simple inclusion of an additional site coupled with the bulk interaction with the system. On the other hand, for $\theta \to \infty$ one obtains an impurity spin totally decoupled from the host. The isotropic antiferromagnetic Heisenberg limit [17] can be easily obtained by the rescaling $\theta, \gamma \to 0$ with $\theta/\gamma = \theta'$ fixed.

The coupling of the impurity to the host (J_{imp}) is determined by the constant θ. It was shown [19, 21] that precisely this constant determines the effective Kondo temperature of the impurity in a spin chain via $T_K \propto \exp(-\pi|\theta|)$. For energies higher than this crossover Kondo scale, one has the asymptotically free impurity spin $\frac{1}{2}$, while for lower energies the impurity spin is screened, and the usual (marginal) FL-like behaviour persists with finite susceptibility and linear temperature dependence of the specific heat at low temperature, and hence finite Wilson ratio in the ground state [4]. This is similar to the findings in the theory of a Kondo impurity in a host of fermions with spin [2]. In other words, θ measures the shift off the Kondo resonance (higher values of $|\theta|$ correspond to lower values on the Kondo scale) of the impurity level with the host spin excitations—similar to the standard picture of the Kondo effect in the electron host. The difference between the two models is simply that in the free-electron host, the spins of free electrons screen the magnetic impurity, while in the spin chain, the low-lying spin excitations (spinons for the antiferromagnetic chain) quench the spin of the impurity.

We can independently incorporate any number of such impurities into the host chain; each of them will be characterized by its own coupling to the host, i.e. by its own θ_j. Hence we obtain an ensemble of spin-$\frac{1}{2}$ impurities with their own Kondo temperatures. The lattice Hamiltonian (1) has additional terms, which renormalize the coupling between the neighbouring sites of the host, and three-spin terms. However, it was shown [21] that in the long-wavelength limit such

a lattice form of the impurity Hamiltonian yields the well-known form of the contact impurity–host interaction, similar that of the usual Kondo problem [2]. The contact impurity coupling in this (conformal) limit is also determined by the same constant θ. We also point out that it was shown that the magnetic behaviour of the impurities in the bulk and the magnetic behaviour of the impurity situated at the edge of the chain (where the renormalization of the coupling between the neighbouring sites of the host and three-spin terms can be eliminated, and the only interaction between the impurity and the host is the standard two-spin exchange interaction) coincide [19, 22]. Finally, we would like to note that all our impurities are *elastic* scatterers, i.e. each excitation only changes its phase when scattering off each impurity, but is not reflected. However, the same property holds for the standard Kondo impurity in a free-electron host [2]. Equally important to mention is that we study a *lattice* model; hence all two-particle scattering processes, in particular from one Fermi point to the other (backscattering), are taken into account in our work. However, we emphasize again that our model (as well as the exact solution for the Kondo problem in metals [2]) does not describe reflecting impurities.

For our one-dimensional quantum spin Hamiltonian at finite temperature, we found a suitable lattice path integral representation by a mapping preserving integrability. For a general formulation of Trotter–Suzuki decompositions the reader is referred to reference [24]. Let $R^{\mu_i\mu_{i+1}}_{\alpha_i\beta_i}(u)$ be the standard R-matrix of the XXZ spin-$\frac{1}{2}$ chain with uniaxial 'easy-plane' anisotropy [23]. Here indices α_i and β_i denote states of the spin at site i, and μ denotes states in the auxiliary space. The 'standard' transfer matrices (row-to-row from the viewpoint of statistical 2D problems) $\tau^{\beta}_{\alpha}(u)$ have the form of the trace over the auxiliary space of the product of R-matrices:

$$\tau^{\beta}_{\alpha}(u, \{\theta\}_{i=1}^{L}) = \sum_{\mu} \prod_{i=1}^{L} R^{\mu_i\mu_{i+1}}_{\alpha_i\beta_i}(u, \theta_i) \tag{2}$$

where L is the length of the quantum chain and θ_i are the inhomogeneity parameters, which are shifts of the spectral parameter. The R-matrices satisfy the Yang–Baxter equations; hence the transfer matrices with different spectral parameters commute. The above-formulated Hamiltonian of the uniaxial spin-$\frac{1}{2}$ quantum chain with impurities is obtained as the derivative of the logarithm of the transfer matrix with respect to the spectral parameter (at $u = 0$). The Hamiltonian and other integrals of motion, which can be constructed in a similar way as higher-order logarithmic derivatives, commute with the transfer matrix. One can introduce R-matrices of different type, related to the initial one by an anticlockwise rotation $\bar{R}^{\mu\nu}_{\alpha\beta}(u) = R^{\alpha\beta}_{\nu\mu}(u)$ and $\tilde{R}^{\mu\nu}_{\alpha\beta}(u) = R^{\beta\alpha}_{\mu\nu}(u)$ by clockwise rotation. The transfer matrix $\bar{\tau}(u, \{\theta\}_{i=1}^{L})$ can be constructed in a way similar to the case for τ. Then we substitute $u = -J \sin\gamma/NT$, where N is the Trotter number. We find

$$[\tau(u)\bar{\tau}(u)]^{N/2} = \mathrm{e}^{-\mathcal{H}/T+\mathcal{O}(1/N)}. \tag{3}$$

Hence, the partition function of the quantum 1D system is identical to the partition function of an inhomogeneous classical vertex model with alternating rows on a square lattice of size $L \times N$:

$$Z = \lim_{N\to\infty} \mathrm{Tr}[\tau(u)\bar{\tau}(u)]^{N/2}. \tag{4}$$

The interactions on the 2D lattice are four-spin interactions with coupling parameters depending on $(NT)^{-1}$ and interaction parameters θ_i where i is the number of the column to which the vertex of the lattice considered belongs to. Note that the interactions are homogeneous in each column, but vary from column to column. We study this system in the limit $N, L \to \infty$ using an approach which is based on a transfer matrix describing transfer in the horizontal direction. The corresponding column-to-column transfer matrices are referred to as 'quantum

transfer matrices' (QTM) (where an external magnetic field H is included by means of twisted boundary conditions):

$$\tau_{QTM}(\theta_j, u) = \sum_{\mu} \mathrm{e}^{\mu_1 H/T} \prod_{i=1}^{N/2} R^{\mu_{2i-1}\mu_{2i}}_{\alpha_{2i-1}\beta_{2i-1}}(u + \mathrm{i}\theta_j) \times \tilde{R}^{\mu_{2i}\mu_{2i+1}}_{\alpha_{2i}\beta_{2i}}(u - \mathrm{i}\theta_j). \tag{5}$$

See figure 1 for an illustration of the model.

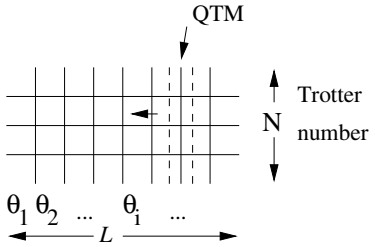

Figure 1. An illustration of the geometry underlying the classical model with four-spin interaction around vertices and alternating coupling parameters from column to column.

In general all QTMs corresponding to the L columns are different. However, all these operators can be proven to commute pairwise. Therefore, the free energy per lattice site of our system can be calculated from just the largest eigenvalues of the quantum transfer matrices (corresponding to only one eigenstate). The free energy per site f of the 1D inhomogeneous quantum XXZ chain is given simply by the largest eigenvalue of the quantum transfer matrix Λ_{QTM}:

$$f = -\lim_{L\to\infty} \frac{T}{L} \sum_{i=1}^{L} \lim_{N\to\infty} \ln \Lambda_{QTM}(\theta_i, u) \tag{6}$$

where

$$u = -\frac{J \sin\gamma}{TN}$$

and the dependence on N is understood implicitly. For a discussion of the homogeneous case, see references [25, 26] and references therein.

By means of a Bethe *ansatz*, we find the eigenvalue of the quantum transfer matrix to be given by

$$\Lambda_{QTM}(\theta_i) = \frac{\Lambda(\theta_i')}{(\sinh(\mathrm{i}\gamma))^N} \tag{7}$$

with $\theta_i = (\gamma/2)\theta_i'$ and

$$\begin{aligned} \Lambda(x) &= \lambda_1(x) + \lambda_2(x) \\ \lambda_1(x) &= \phi_+(x)\phi_-(x - 2\mathrm{i})\mathrm{e}^{H/T} \frac{Q(x + 2\mathrm{i})}{Q(x)} \\ \lambda_2(x) &= \phi_-(x)\phi_+(x + 2\mathrm{i})\mathrm{e}^{-H/T} \frac{Q(x - 2\mathrm{i})}{Q(x)}. \end{aligned} \tag{8}$$

Here we have dropped the dependence on u and θ_i, which are fixed, and consider the dependence on the spectral parameter x explicitly. Furthermore, we have used

$$\phi_\pm(x) = \sinh\frac{\gamma}{2}(x \pm \mathrm{i}u') \qquad Q(x) = \prod_{j=1}^{m} \sinh\frac{\gamma}{2}(x - x_j)$$

with 'renormalized' $u = (\gamma/2)u'$. Here $\{x_j\}_{j=1}^{m}$ is the set of Bethe *ansatz* rapidities which are subject to the Bethe *ansatz* equations [25, 26]. For the largest eigenvalue, one has to take $m = N/2$. However, we will not solve the Bethe *ansatz* equations directly, but rather will be interested in the functional properties of the eigenvalue of the transfer matrix. For this purpose we introduce four auxiliary functions $b(x)$, $\bar{b}(x)$, $B(x) = 1 + b(x)$ and $\bar{B}(x) = 1 + \bar{b}(x)$ as follows:

$$\begin{aligned} b(x) &= \lambda_1(x + \mathrm{i})/\lambda_2(x + \mathrm{i}) \\ \bar{b}(x) &= \lambda_2(x - \mathrm{i})/\lambda_1(x - \mathrm{i}). \end{aligned} \tag{9}$$

Then one can straightforwardly check that

$$\begin{aligned} \Lambda(x + \mathrm{i}) &= B(x)\lambda_2(x + \mathrm{i}) = \mathrm{e}^{-H/T} \prod_{\pm} \phi_{\pm}(x + 2\mathrm{i} \pm \mathrm{i}) \frac{Q(x - \mathrm{i})}{Q(x + \mathrm{i})} \\ \Lambda(x - \mathrm{i}) &= \bar{B}(x)\lambda_1(x - \mathrm{i}) = \mathrm{e}^{H/T} \prod_{\pm} \phi_{\pm}(x - 2\mathrm{i} \pm \mathrm{i}) \frac{Q(x + \mathrm{i})}{Q(x - \mathrm{i})}. \end{aligned} \tag{10}$$

Obviously

$$\begin{aligned} b(x) &= \mathrm{e}^{2H/T} \prod_{\pm} \frac{\phi_{\pm}(x \pm \mathrm{i})}{\phi_{\pm}(x + 2\mathrm{i} \pm \mathrm{i})} \frac{Q(x + 3\mathrm{i})}{Q(x - \mathrm{i})} \\ \bar{b}(x) &= \mathrm{e}^{-2H/T} \prod_{\pm} \frac{\phi_{\pm}(x \pm \mathrm{i})}{\phi_{\pm}(x - 2\mathrm{i} \pm \mathrm{i})} \frac{Q(x - 3\mathrm{i})}{Q(x + \mathrm{i})}. \end{aligned} \tag{11}$$

One can see that these auxiliary functions are analytic, non-zero, and have constant asymptotic behaviour for the strip $-1 < \operatorname{Im} x \leqslant 0$ for $b(x)$ and $B(x)$, and for the strip $0 \leqslant \operatorname{Im} x < 1$ for $\bar{b}(x)$ and $\bar{B}(x)$. Introducing

$$a(x) = b\left(\frac{2}{\pi}(x + \mathrm{i}\epsilon)\right) \qquad \bar{a}(x) = \bar{b}\left(\frac{2}{\pi}(x - \mathrm{i}\epsilon)\right)$$

(infinitesimal $\epsilon > 0$), taking the logarithmic derivative of these functions, Fourier transforming the equations, eliminating the functions $Q(x)$, and then inverse Fourier transforming, we obtain the final set of two non-linear integral equations. Eventually, we take the limit $N \to \infty$. Proceeding in this way, we find for our system the following set of non-linear integral equations for the 'energy-density' functions of spinons a, $\bar{a}$, $A = 1 + a$, and $\bar{A} = 1 + \bar{a}$, depending on the spectral parameter x:

$$\begin{aligned} \ln a(x) = &-\frac{v}{T \cosh x} + \frac{\pi h}{2(\pi - \gamma)T} \\ &+ \int \left[k(x - y) \ln A(y) - k(x - y - \pi\mathrm{i} + \mathrm{i}\epsilon) \ln \bar{A}(y)\right] \mathrm{d}y \end{aligned} \tag{12}$$

with

$$v = \pi \frac{\sin \gamma}{\gamma}$$

and the kernel function

$$k(x) = \frac{1}{2\pi} \int \mathrm{d}\omega \left\{ \sinh\left[\left(\frac{\pi^2}{2\gamma} - \pi\right)\omega\right] \cos(x\omega) \right\} \Big/ \left\{ 2 \cosh\left(\frac{\pi\omega}{2}\right) \sinh\left(\frac{\pi - \gamma}{2\gamma}\pi\omega\right) \right\}. \tag{13}$$

The corresponding equation for $\bar{a}(x)$ is obtained from equation (12) by making the exchanges $\mathrm{i} \to -\mathrm{i}$, $h \to -h$, and $a, A \leftrightarrow \bar{a}, \bar{A}$. The free energy per site f is given by

$$f(x) = e_0(x) - \frac{T}{2\pi} \int \frac{\ln[A(y)\bar{A}(y)]\, \mathrm{d}y}{\cosh(x - y)} \tag{14}$$

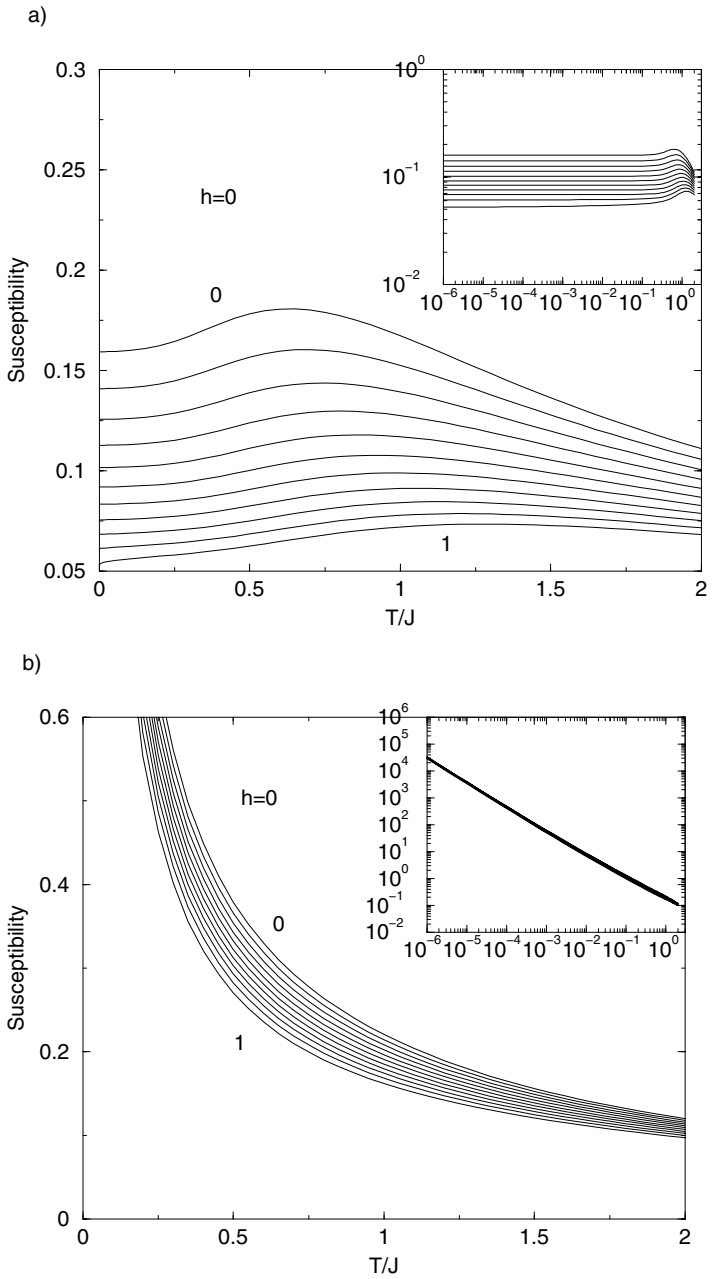

Figure 2. The magnetic susceptibility χ versus temperature T for zero magnetic field and anisotropies $\Delta = 0, 0.1, \ldots, 1$ for: (a) the homogeneous spin chain, (b) Lorentzian distribution, and (c) log-normal distribution. The insets show log–log plots of the data.

where e_0 is the ground-state energy. The free energy of the total chain with impurities is

$$F = \sum_j f\left(\frac{\pi}{2}\theta'_j\right)$$

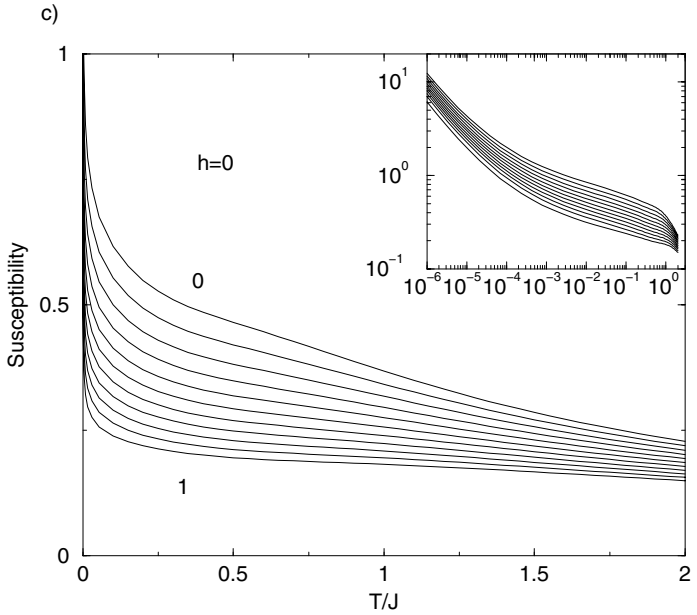

Figure 2. (Continued)

where the sum is taken over all the sites (for sites without impurities we get $f(0)$). These equations are easily solved numerically for arbitrary magnetic field values and temperatures. The random distribution of the values θ_j (or of the Kondo temperatures for the impurities) can be described by a distribution function $P(\theta_j)$.

It is worthwhile to emphasize here the simplicity of the derived equations: for each impurity there is only one parameter, the shift of the spectral parameter in the formula for the free energy per site equation (14). Then the exact solvability of the problem for any number of impurities permits one to introduce the distribution of these shifts (or the strengths of the impurity–host couplings, i.e. the local Kondo temperatures). One has only two (non-linear) integral equations, equations (12), to solve, and the answer can in principle be obtained for arbitrary temperature and magnetic field ranges.

3. Results and discussion

In figures 2 and 3 the results for the magnetic susceptibility and the linear temperature coefficient of the specific heat c/T at zero field and for antiferromagnetic anisotropy ($0 \leqslant \Delta \leqslant 1$) are plotted as functions of temperature for: the homogeneous chain, the Lorentzian distribution† $P(\theta) = (\pi^2 + \theta^2)^{-1}$, and the so-called logarithmically normal [27] distribution

$$P(\theta) = \pi^{-1/2}(|\theta| + 10^{-6})^{-1} \exp\left(-\left[\ln(|\theta| + 10^{-6}) + \frac{1}{4}\right]^2\right)$$

which is characteristic for strong disorder, e.g. close to a critical point [12]). Note that the Gaussian and the logarithmically normal distributions can be considered as two limiting cases (for narrow and wide distributions) of a more general distribution [27]. One can observe a clear qualitative difference between strong disorder (Lorentzian and log-normal) and the pure

† Here we are dealing with distributions in the rescaled θ', but drop $'$ for simplicity.

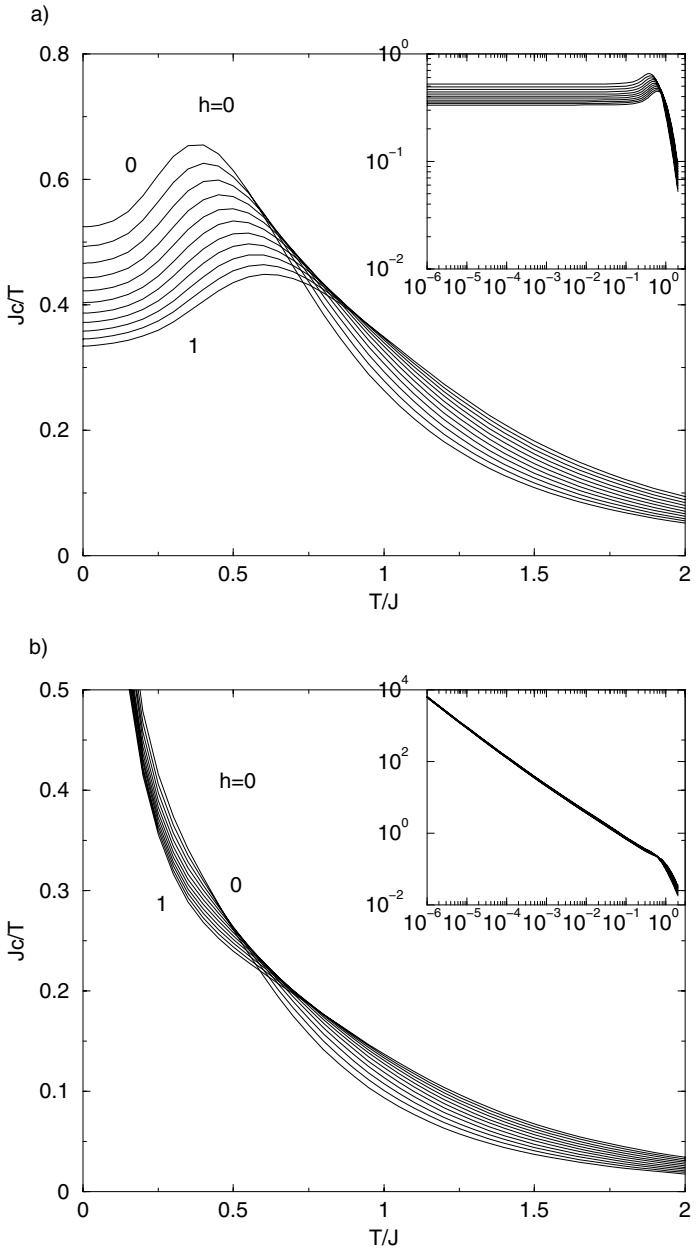

Figure 3. The reduced specific heat c/T versus temperature T for zero magnetic field and anisotropies $\Delta = 0, 0.1, \ldots, 1$ for: (a) the homogeneous spin chain, (b) Lorentzian distribution, and (c) log-normal distribution. The insets show log–log plots of the data.

curve. For the pure system we have finite low-temperature limits of χ and c/T. Note that $\chi(T)$ (figure 2) takes smaller values for larger Δ, i.e. stronger antiferromagnetic anisotropy. Also in figure 2(a) an infinite slope of $\chi(T)$ at $T = 0$ and $\Delta = 1$ due to logarithmic corrections is visible. For Lorentzian disorder we find algebraically divergent χ and c/T with effective exponents ranging from 0.91 to 0.92 for $\Delta = 0$ to 1 (χ), and from 0.826

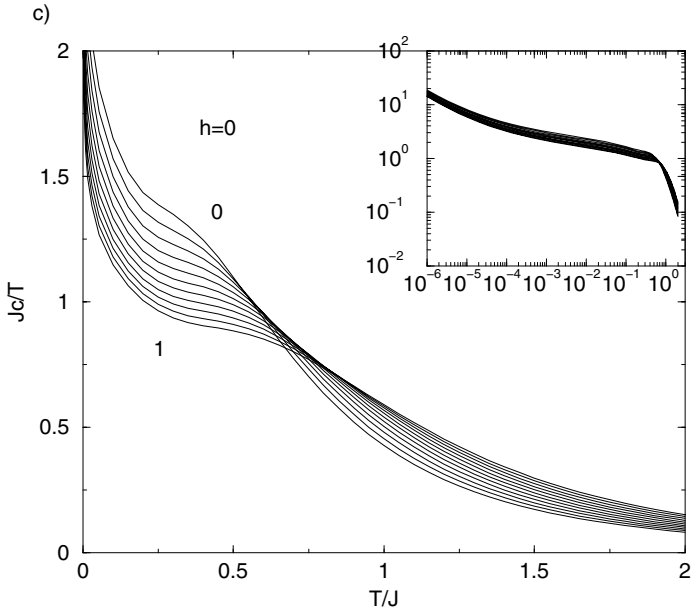

Figure 3. (Continued)

to 0.833 for $\Delta = 0$ to 1 (c/T), respectively. These numbers differ a little from those quoted in [17] as we fitted the rather low-temperature region $10^{-6}J < T < 5 \times 10^{-4}J$ in the present work. Note that usually for low-dimensional quantum magnets the exchange constant $J \sim 10^2$–10^3 K [31, 32] (for heavy fermions the corresponding constant, the width of the band, is 10^4–10^5 K [5, 6, 8–10, 14, 30]); hence our temperature interval more than covers the range of temperatures of experiments (usually 10^{-1}–10 K [5, 6, 8–10, 14, 30]). The temperature dependence of the effective exponents is small in the Lorentzian case. The origin of these variations is revealed in a more detailed study of the low-temperature asymptotics by logarithmic correction terms. In the case of Lorentzian disorder we have

$$c \sim \{\log(1/T)\}^{-2} \qquad \chi \sim \{T \log(1/T)\}^{-1}.$$

The temperature dependence of the effective exponents for the logarithmically normal distribution is much larger. Here we find the following low-temperature asymptotics:

$$c \sim \{\log(1/T) \exp([\log\log(1/T)]^2)\}^{-1}$$

and

$$\chi \sim \{T \log\log(1/T) \exp([\log\log(1/T)]^2)\}^{-1}.$$

We point out the weaker divergences of the log-normal case compared to the Lorentzian one.

Our results for the low-temperature thermodynamics are close to those of the perturbative calculations of random AF spin-$\frac{1}{2}$ chains [28, 29]: χ and c/T have weak power-law or logarithmic singularities. Our low-temperature results confirm the weak dependence of the critical exponents on temperature. The rather large deviations of the exponents for χ and c/T are due to strong logarithmic corrections at low temperatures for the strongly disordered systems. For an illustration of this effect see also figure 4 showing the Wilson ratios $c/T\chi$ which are non-universal, i.e. with NFL behaviour, and show infinite slope at $T = 0$. In the strongly disordered cases we have at low temperatures

$$c/T\chi \sim 1/\{\log(1/T)\}$$

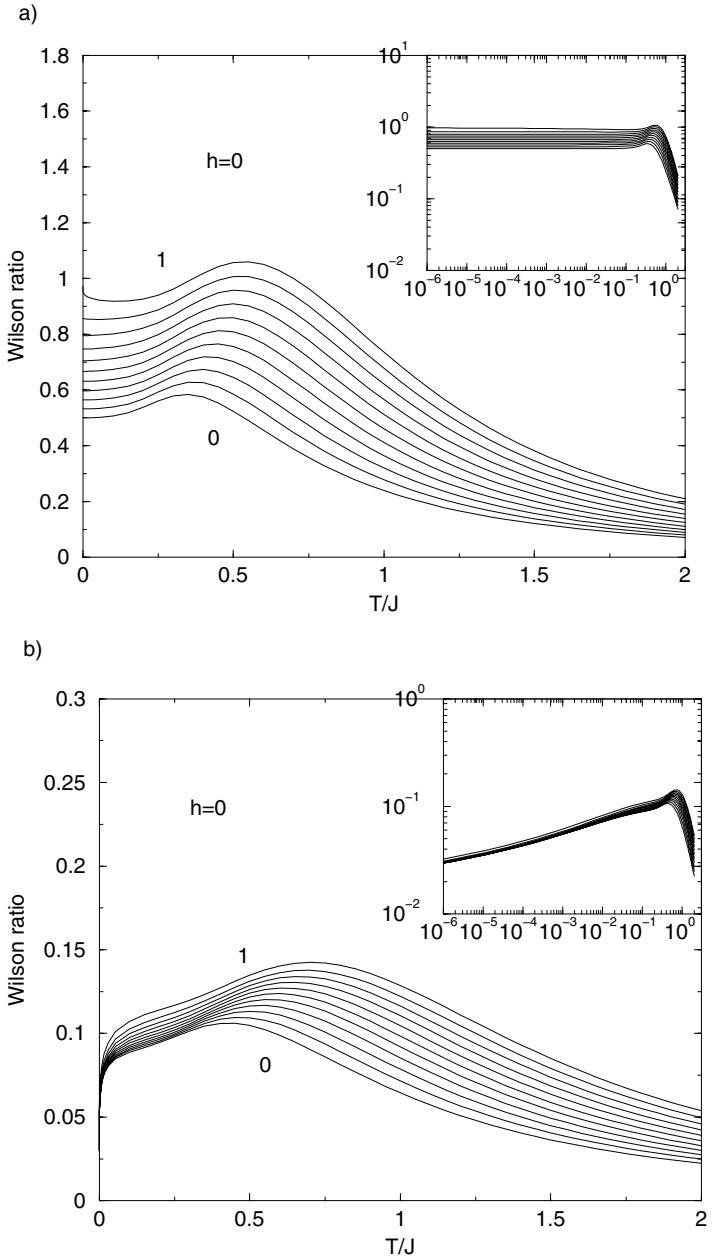

Figure 4. The Wilson ratio [2] $Jc/T\chi$ in units of $2\pi^2/3$ versus temperature T at zero magnetic field and anisotropies $\Delta = 0, 0.1, \ldots, 1$ for: (a) the homogeneous spin chain, (b) Lorentzian distribution, and (c) log-normal distribution. The insets show log–log plots of the data. Note the infinite slope at $T = 0$ in the cases (b) and (c).

(Lorentz) and

$$c/T\chi \sim \log\log(1/T)/\{\log(1/T)\}$$

(log-normal). Even in the pure case we have infinite slope for $\Delta = 1$, however with finite

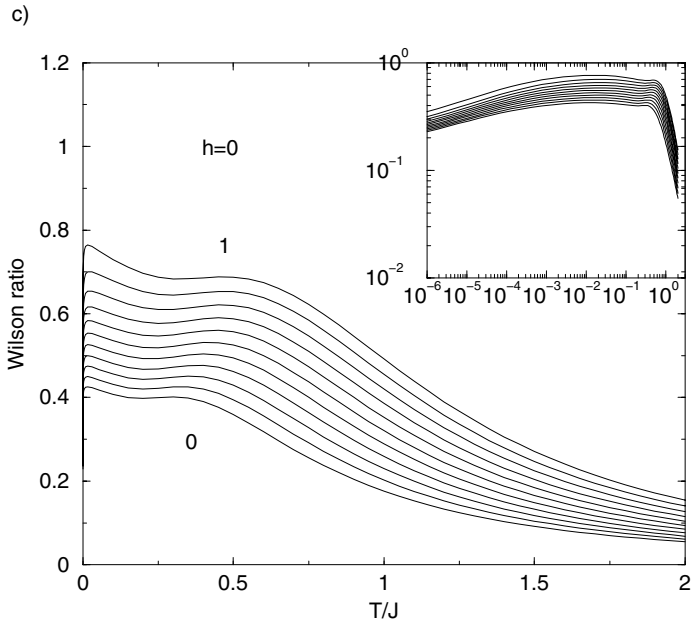

Figure 4. (Continued)

zero-temperture limit. For the general homogeneous case the zero-temperature limit of the Wilson ratio is $2\pi(\pi - \gamma)/3$ where γ is given by the anisotropy $\Delta = \cos\gamma$.

We point out that the infinite slope at $T = 0$ for the homogeneous Heisenberg chain is due to the known logarithmic singularities (see e.g. [26] and references therein). They are only present for the case $\Delta = 1$.

It turns out that for weak disorder (with narrow distribution of θ), for instance the Gaussian distribution (in θ), the effective Kondo temperature of the ensemble of the impurities is higher than the applied temperature, and hence the impurities are quenched by the host spin chain with (marginal) FL-like behaviour of the thermodynamic characteristics: finite susceptibility and Wilson ratio, linear temperature dependence of the specific heat at low temperatures [4]. However, we point out that even for weak disorder the thermodynamic characteristics (susceptibility and specific heat) at low temperatures take larger values than in the homogeneous case, see figure 5.

It is clear that the divergent value of the magnetic susceptibility at low T for strong disorder (with wide distributions in θ) of the impurity–host couplings is connected with the fact that for most of the impurities their Kondo temperatures are lower than the temperature of the system. Therefore these impurities give rise to a Curie-like behaviour of the susceptibility. This divergence disappears upon applying a finite external field which restores most of the (marginal) FL-like behaviour; see figures 6, 7.

We would like to note that the former calculations were valid at most for low temperatures, while our non-linear equations are applicable to *any* temperature and magnetic field scales. Furthermore, it is also known that the approximate results [28, 29] incorrectly give zero or infinite susceptibility at $T \to 0$ irrespective of the distribution, while its true value is finite for e.g. the homogeneous chain and the single impurity [19, 26]. Our scheme, of course, perfectly describes the correct behaviour. We also performed a comparison of our results with the data of reference [8], finding qualitatively similar results. Note that any distribution

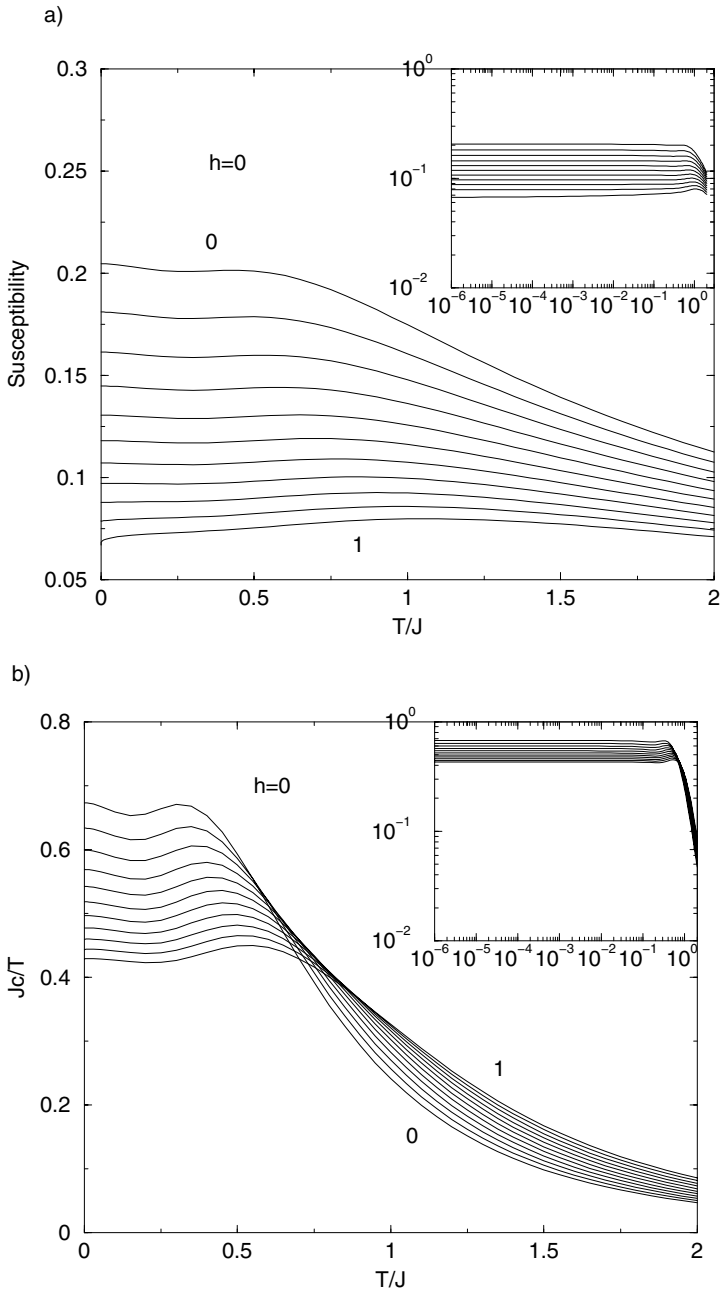

Figure 5. Gaussian distribution: depiction of (a) the magnetic susceptibility χ, (b) the reduced specific heat c/T, and (c) the Wilson ratio [2] $Jc/T\chi$ in units of $2\pi^2/3$ versus temperature T at zero magnetic field and anisotropies $\Delta = 0, 0.1, \ldots, 1$. The insets show log–log plots of the data.

$P(\lambda)$ of impurity couplings λ ($\propto 1/\theta$ in our parametrization) with finite $P(0)$ corresponds to a Lorentzian-like distribution in θ. Hence the agreement of our data with references [8, 13]: infinite χ and $c/T\chi$ for $T \to 0$. The comparison with experiments can be seen more clearly

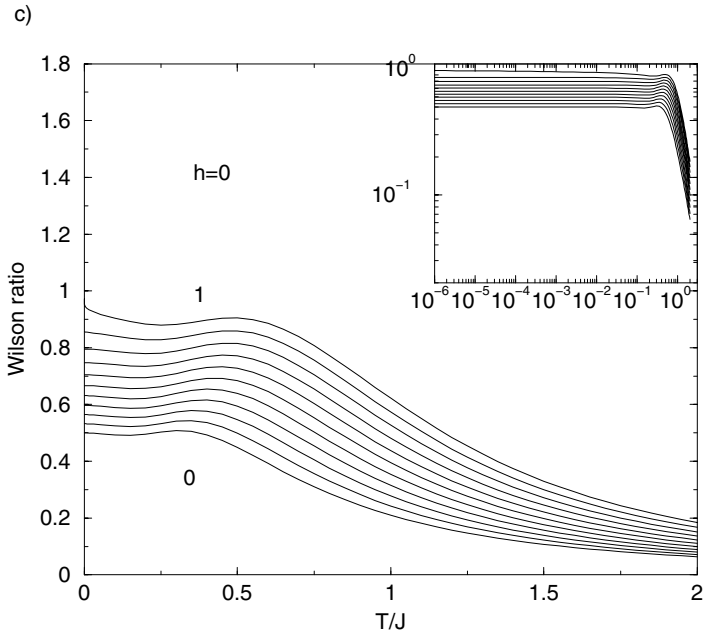

Figure 5. (Continued)

from references [9, 30–32]. By changing the concentration of magnetic impurities, one can go from weak to strong disorder with quantitative agreement with narrow and wide Gaussian and log-normal distributions [30]. Critical exponents close to those of our Lorentzian distribution were observed in references [31, 32] for the experiments on disordered spin-$\frac{1}{2}$ salts of TCNQ. Notice also that the values of the critical exponents depend strongly on the temperature interval for the calculated characteristics: they become larger for the models of strong disorder for lower temperature ranges. Hence for successful comparison with experiments, one needs to know in which temperature window the magnetic susceptibility and specific heat were measured. For example in reference [32] the exchange constant $J = 600$ K, and effective exponents measured at temperatures of the order of 10 K were about 0.7.

See figures 8 and 9 for the case of ferromagnetic anisotropy and zero field. Note that $\chi(T)$ for the pure chain (figure 8(a)) takes growing values for Δ approaching -1, i.e. for increasingly ferromagnetic anisotropy. This behaviour may be expected intuitively; however, in the strongly disordered cases (b) and (c), this property only holds at higher temperatures, and an inversion takes place at some lower temperature. In the logarithmically disordered case (c), some plateau-like structures in the log–log plot seem to appear; however, at sufficiently low temperatures the expected divergence sets in. Note that for $\Delta < -0.5$ the plateau region extends down to the lowest temperature treated, $10^{-6}J$. For the Lorentzian disorder we find algebraically divergent χ and c/T with effective exponents ranging from 0.91 to 0.85 for $\Delta = 0$ to -0.9 (χ), and from 0.826 to 0.746 for $\Delta = 0$ to -0.9 (c/T), respectively. Note that these exponents are smaller than those in the case of antiferromagnetic anisotropy, and also show a larger spread. The differences between the behaviour of the Kondo-like screening for the disordered impurities in the antiferromagnetic and ferromagnetic 'easy-plane' chains are probably connected with the fact that the ground state (and thus the low-temperature properties) of the former corresponds to the filling of the Dirac sea for spinons which carry spin $\frac{1}{2}$. On the other hand, as we get closer to the isotropic ferromagnetic case, the influence

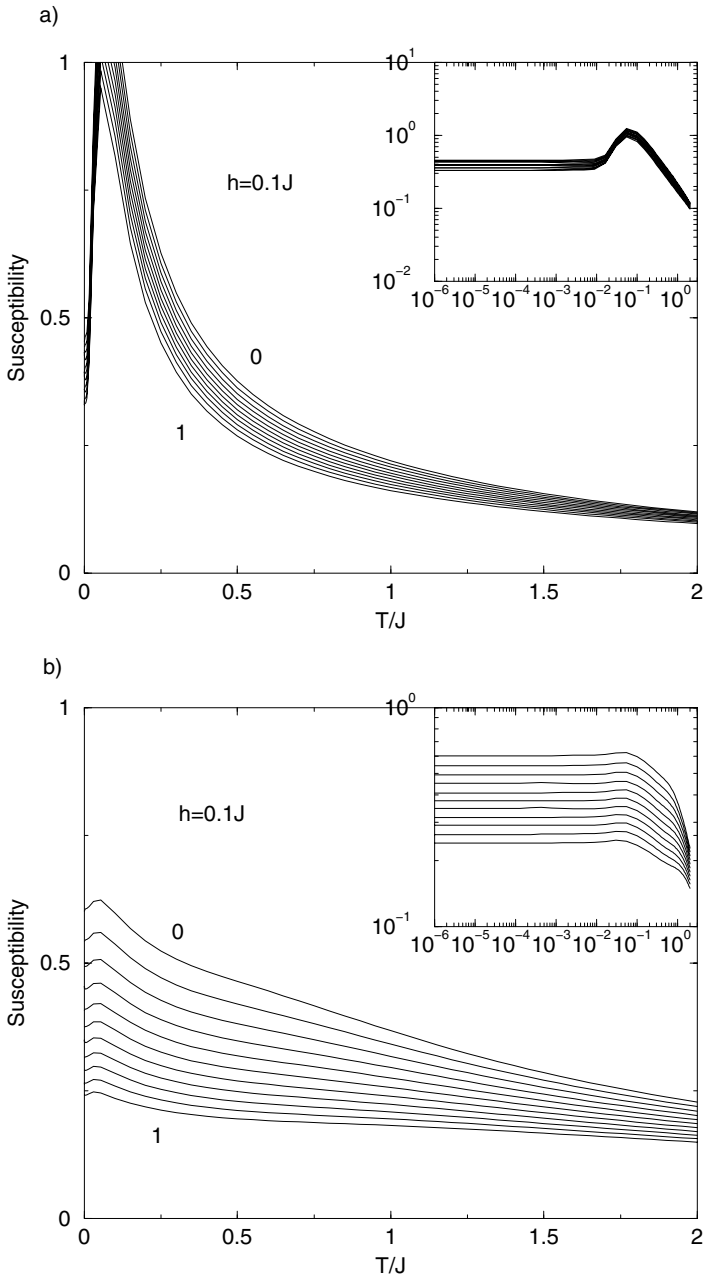

Figure 6. The magnetic susceptibility χ versus temperature T for the magnetic field $h = 0.1J$ and anisotropies $\Delta = 0, 0.1, \ldots, 1$ for: (a) Lorentzian distribution, and (b) log-normal distribution. The insets show log–log plots of the data.

of the spin complexes of greater length (bound states), carrying higher spin, becomes more pronounced. That is why the spins of the impurities in such a situation are screened by the low-lying excitations of the host which carry spin higher than $\frac{1}{2}$, similarly to the situation in the multichannel Kondo problem [4].

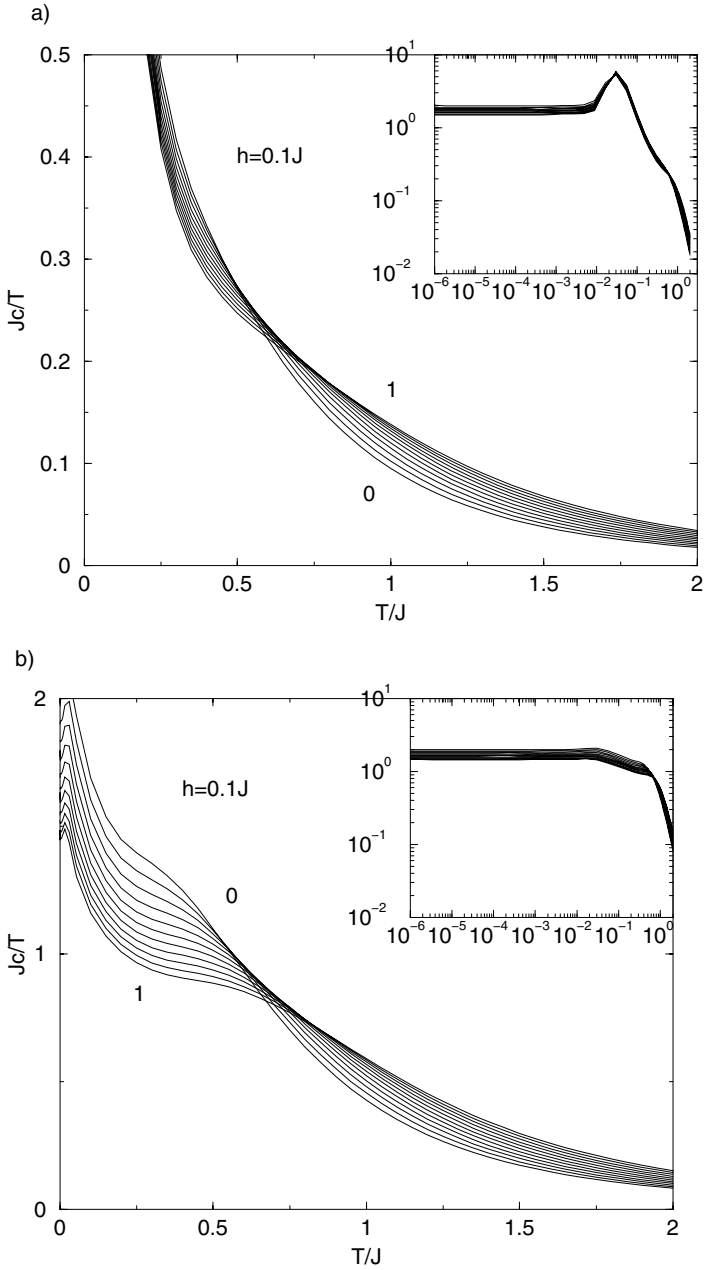

Figure 7. The reduced specific heat c/T versus temperature T for the magnetic field $h = 0.1J$ and anisotropies $\Delta = 0, 0.1, \ldots, 1$ for: (a) Lorentzian distribution, and (b) log-normal distribution. The insets show log–log plots of the data.

Generalizing model (1) but keeping the exact solvability, it is possible to include (random) short- and long-range antiferromagnetic interactions of special form between the impurities themselves; see e.g. references [20,33]. However, these interactions do not affect the behaviour of our disordered correlated spin system qualitatively compared to the case without direct

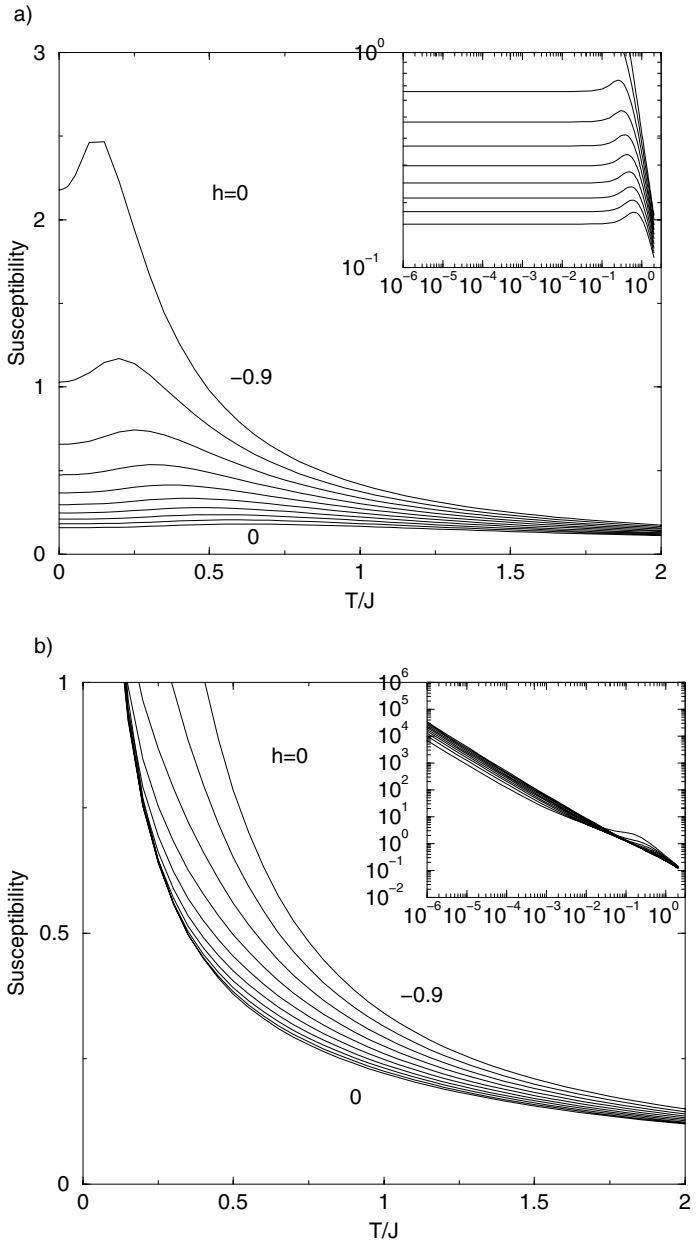

Figure 8. The magnetic susceptibility χ versus temperature T for zero magnetic field and anisotropies $\Delta = 0, -0.1, \ldots, -0.9$ for: (a) the homogeneous spin chain, (b) Lorentzian distribution, and (c) log-normal distribution. The insets show log–log plots of the data.

interaction between impurities. Here, a probability distribution $P(\theta)$ with asymptotics $|\theta|^{-\alpha'}$ for large θ leads to a divergence $\chi(T) \propto T^{-1/\alpha'}$ which is weaker than that observed above. It was suggested [15] that the inclusion of other kinds of impurity–impurity couplings (of RKKY long-range form, which violate exact integrability) also do not change the behaviour qualitatively. However, ferromagnetic impurity–impurity couplings in the antiferromagnetic

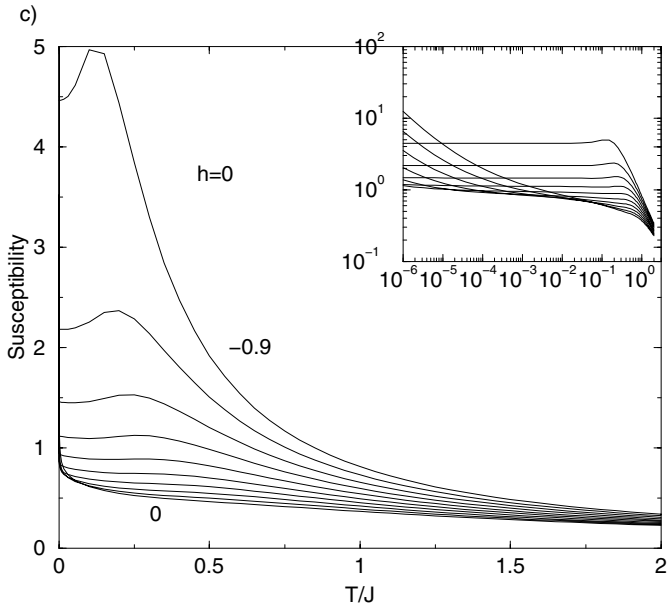

Figure 8. (Continued)

host and vice versa can change the situation drastically, e.g. providing infinite $\chi(T \to 0)$ even for weak disorder.

The generalization of our results to correlated electron systems with random impurities will be reported elsewhere.

4. Concluding remarks

To conclude, we have constructed exactly the thermodynamics of the 'easy-plane' uniaxial spin-$\frac{1}{2}$ quantum chain with embedded disordered impurities. To the best of our knowledge, this is the first example where a model with disorder as well as strong correlations in the host (i.e. disorder in the strongly interacting many-body problem) has been solved exactly for a wide range of temperatures and external fields.

The results are of high (numerical) accuracy and valid for arbitrary ranges of magnetic field and temperature. We have shown that for strong disorder (wide distribution) of the impurity–host couplings, the local moments of the impurities are non-quenched by the excitations of the critical uniaxial antiferromagnetic spin chain. For weak disorder of the host–impurity couplings, on the other hand, spin excitations of the host screen the impurities, but with non-Fermi-liquid behaviour of the thermodynamic characteristics (the temperature interval with Fermi-liquid-like behaviour becomes very narrow). The external magnetic field lifts the degeneracy, hence supporting the screening of the impurity. The 'easy-plane' anisotropy in the antiferromagnetic chain (which does not drive the host system out of the critical region) does not drastically change the behaviour of the disorder compared with the isotropic case, but weakly renormalizes the exponents for the low-temperature magnetic susceptibility and specific heat. In contrast, the same type of anisotropy but in the ferromagnetic host for not very strong disorder 'restores' the quenching of the impurities by the host for intermediate temperatures. However, very strong disorder (like the Lorentzian distribution of the impurity–host couplings)

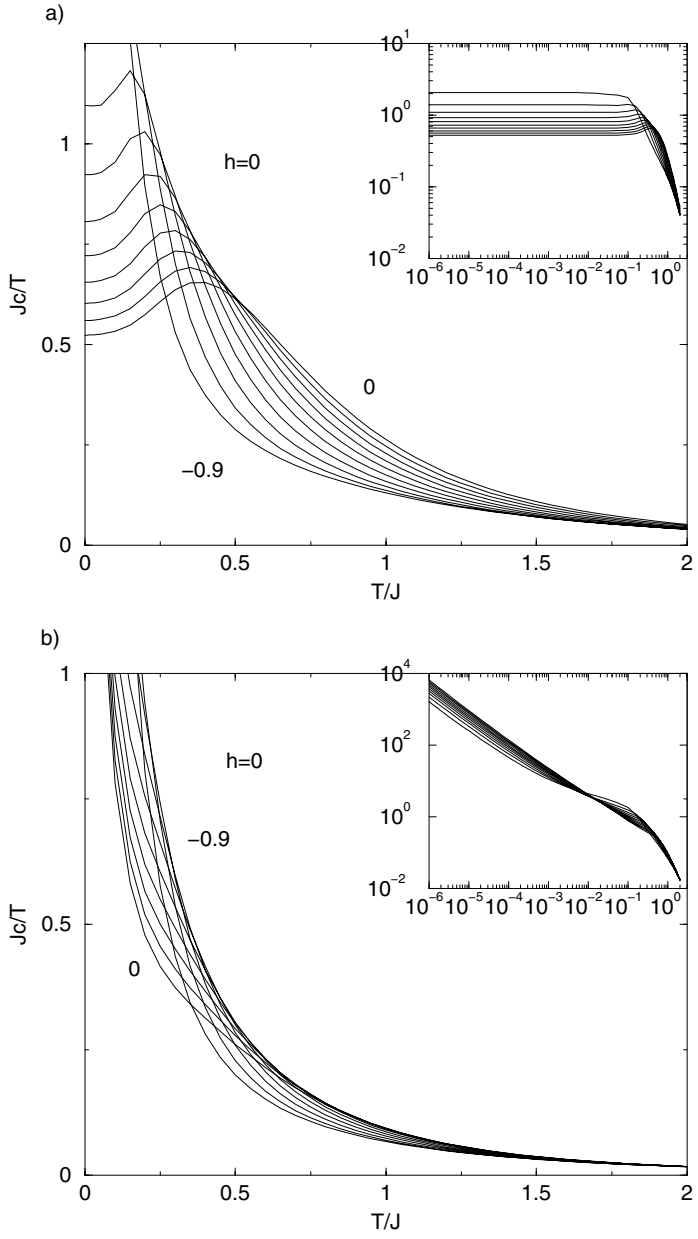

Figure 9. The reduced specific heat c/T versus temperature T for zero magnetic field and anisotropies $\Delta = 0, -0.1, \ldots, -0.9$ for: (a) the homogeneous spin chain, (b) Lorentzian distribution, and (c) log-normal distribution. The insets show log–log plots of the data.

manifests the lower degree of screening and the divergent asymptotics of the specific heat and susceptibility for $T \to 0$. We relate such a different behaviour to the stronger influence of the spinon bound states, carrying larger spin values, on the low-temperature properties of the disordered spin chains with ferromagnetic anisotropy.

We performed a comparison of our theory with the data from a perturbative analysis,

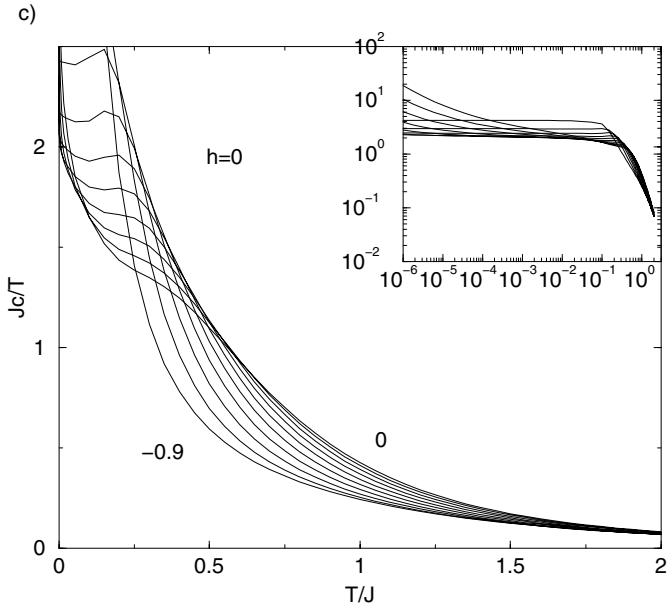

Figure 9. (Continued)

finding striking agreement for the case of strong disorder. Note, however, that in the case of weak disorder the perturbative analysis yields an unphysical divergence of the susceptibility, whereas our data correctly reproduce the absence of such divergences. We also compared our results with those of magnetic experiments on disordered spin chains and disordered non-Fermi liquids in rare-earth alloys. This comparison reveals good qualitative agreement.

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References

[1] See, e.g.,
Kondo J 1969 *Solid State Physics: Advances in Research and Applications* vol 23, ed F Seitz, D Turnbull and H Ehrenreich (New York: Academic) p 184

[2] Andrei N, Furuya K and Lowenstein J H 1983 *Rev. Mod. Phys.* **55** 331
Tsvelick A M and Wiegmann P B 1983 *Adv. Phys.* **32** 453

[3] For a recent review of the bosonization approach to the Kondo problem, see
Affleck I 1995 *Acta Phys. Pol.* B **26** 1869

[4] Schlottmann P and Sacramento P D 1993 *Adv. Phys.* **42** 641

[5] For recent review of the non-Fermi-liquid behaviours, see
von Löhneysen H, Huster F, Mock S, Neubert A, Pietrus T, Sieck M, O Stockert and Waffenschmidt M M 1997 *Physica* B **230–232** 550

[6] For recent review of non-Fermi-liquid behaviours, see
Maple M B, de Andrade M C, Herrmann J, Dalichaouch Y, Gajewski D A, Seaman C L, Chau R, Movshovich R, Aronson M C and Osborn R 1995 *J. Low Temp. Phys.* **99** 223

[7] Seaman C, Maple M B, Lee B W, Ghamaty S, Torikachvili M S, Kang J-S, Liu L Z, Allen J W and Cox D L 1991 *Phys. Rev. Lett.* **67** 2882
Stewart G R 1993 *Phys. Rev.* B **47** 3208
Aronson M C, Osborn R, Robinson R A, Lynn J W, Chau R, Seaman S L and Maple M B 1995 *Phys. Rev. Lett.* **75** 725
Andraka B 1994 *Phys. Rev.* B **49** 348
Andraka B 1994 *Phys. Rev.* B **49** 3589
[8] Bernal O O, MacLaughlin D E, Lukefahr H G and Andraka B 1995 *Phys. Rev. Lett.* **75** 2023
[9] de Andrade M C, Chau R, Dickey R P, Dilley N R, Freeman E J, Gajewski D A, Maple M B, Movshovich R, Castro Neto A H, Castilla G E and Jones B A 1998 *Phys. Rev. Lett.* **81** 5620
[10] Booth C H, MacLaughlin D E, Heffner R H, Chau R, Maple M B and Kwei G H 1998 *Phys. Rev. Lett.* **81** 3960
[11] Bhatt R N and Fisher D S 1992 *Phys. Rev. Lett.* **68** 3072
[12] Dobrosavljević V, Kirkpatrick T R and Kotliar G 1992 *Phys. Rev. Lett.* **69** 1113
[13] Miranda E, Dobrosavljević V and Kotliar G 1997 *Phys. Rev. Lett.* **78** 290
Miranda E, Dobrosavljević V and Kotliar G 1996 *J. Phys.: Condens. Matter* **8** 9871
[14] MacLaughlin D E, Heffner R H, Nieuwenhuys G J, Luke G M, Fudamoto Y, Uemura Y J, Chau R, Maple M B and Andraka B 1998 *Phys. Rev.* B **58** R11 849
[15] Castro Neto A H, Castilla G and Jones B A 1998 *Phys. Rev. Lett.* **81** 3531
[16] Rajan V J 1983 *Phys. Rev. Lett.* **51** 308
[17] Klümper A and Zvyagin A A 1998 *Phys. Rev. Lett.* **81** 4975
[18] Andrei N and Johannesson H 1984 *Phys. Lett.* A **100** 108
[19] Frahm H and Zvyagin A A 1997 *J. Phys.: Condens. Matter* **9** 9939
[20] Schlottmann P 1994 *Phys. Rev.* B **49** 9202
Zvyagin A A and Schlottmann P 1995 *Phys. Rev.* B **52** 6569
[21] Zvyagin A A and Schlottmann P 1997 *J. Phys.: Condens. Matter* **9** 3543
Zvyagin A A and Schlottmann P 1997 *J. Phys.: Condens. Matter* **9** 6479 (erratum)
[22] Zvyagin A A 1997 *Phys. Rev. Lett.* **79** 4641
[23] See, e.g., the monograph
Korepin V E, Bogoliubov N M and Izergin A G 1993 *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge: Cambridge University Press) and references therein
[24] Suzuki M and Inoue M 1987 *Prog. Theor. Phys.* **78** 787
[25] Klümper A 1992 *Ann. Phys., Lpz.* **1** 540
Klümper A 1993 *Z. Phys.* B **91** 507
[26] Klümper A 1998 *Euro. Phys. J.* B **5** 677
[27] See, e.g.,
Al'tshuler B L and Prigodin V N 1987 *Pis. Zh. Eksp. Teor. Fiz.* **45** 538 (Engl. Transl. 1987 *JETP Lett.* **45** 687)
[28] Ma S-K, Dasgupta C and Hu C-K 1979 *Phys. Rev. Lett.* **43** 1434
Dasgupta C and Ma S-K 1980 *Phys. Rev.* B **22** 1305
[29] Hirsch J E and José J V 1980 *J. Phys. C: Solid State Phys.* **13** L53
Hirsch J E 1980 *Phys. Rev.* B **22** 5355
[30] Matsuhira K, Sakakibara T and Amitsuka H 1995 *Physica* B **206+207** 326
Shlyk L, Waerenborgh J C, Estrela P, De Long L E, de Visser A and Almeida M 1999 *J. Phys.: Condens. Matter* **11** 3525
[31] Bulaevsky L N, Zvarykina A V, Karimov Yu S, Lyubosky R B and Shchegolev I F 1972 *Zh. Eksp. Teor. Fiz.* **62** 725 (Engl. Transl. 1972 *Sov. Phys.–JETP* **35** 384)
[32] Ikegami K, Kuroda S, Saito M, Saito K, Sugi M, Nakamura T, Matsumoto M and Kawabata Y 1987 *Phys. Rev.* B **35** 3667
[33] Schlottmann P and Zvyagin A A 1997 *Phys. Rev.* B **56** 13989