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Integrable versus non-integrable spin chain impurity models

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Abstract. Recent renormalization group studies of impurities in spin-1/2 chains appear to be inconsistent with Bethe ansatz results for a special integrable model. We study this system in more detail around the integrable point in parameter space and argue that this integrable impurity model corresponds to a non-generic multi-critical point. Using previous results on impurities in half-integer spin chains, a consistent renormalization group flow and phase diagram is proposed.

1. Introduction

Recently there has been considerable interest in various quantum impurity problems [1–5]. These can generally be formulated as one-dimensional Luttinger liquids interacting with local defects of various kinds. In general it is expected that such quantum impurity models renormalize to critical points which correspond to conformally invariant boundary conditions. The quantum impurity is screened and/or decouples; it does not appear in the fixed point Hamiltonian although a remnant effective impurity, decoupled from the continuum degrees of freedom, may be left behind.

A particularly simple example is a single impurity in a spin $S = 1/2$ Heisenberg antiferromagnetic chain. Two of the present authors analysed a large class of models of this type using analytic renormalization group (RG) arguments and numerical finite-size analysis [6]. We concluded that the only stable critical points correspond to a completely unperturbed chain or else a chain with a break at the impurity location. Taking the initial boundary conditions to be periodic, we refer to these two critical points as the periodic and open chain, respectively. In the open case, but not the periodic, a remnant impurity spin may also be present, as we shall review in section 2. It was recently drawn to our attention that a Bethe ansatz integrable impurity model of this type was solved several years ago. Its low-energy behaviour corresponds to a conformally invariant boundary condition, but not to one of the stable critical points mentioned above. The purpose of the present article is to resolve this apparent contradiction.

The integrable impurity model involves a single spin-S impurity which is coupled symmetrically to two neighbouring sites on the chain. The Hamiltonian, found by Andrei and Johannesson [7] is

$$H_{\mathrm{Int}} = \tfrac{1}{4}\sum_{i=1}^{L-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \tfrac{1}{4}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_L + \tfrac{1}{2}\left(\frac{2}{2S+1}\right)^2 \times [\boldsymbol{\sigma}_1 \cdot \boldsymbol{S} + \boldsymbol{\sigma}_L \cdot \boldsymbol{S} + \tfrac{1}{2}\{\boldsymbol{\sigma}_1 \cdot \boldsymbol{S}, \boldsymbol{\sigma}_L \cdot \boldsymbol{S}\} - S(S+1)\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_L]. \qquad (1.1)$$

where the σ_i's are Pauli matrices and $\{,\}$ denotes the anti-commutator. In the following we shall refer to (1.1) as the integrable impurity model. The equivalent problem of a spin-1 chain coupled to a spin-S impurity was solved by Lee and Schlottmann [8], and later generalized to a spin-S' chain coupled to a spin-S impurity [9]. For $S \geqslant S'$ it was found that in the thermodynamic limit the system behaves like a spin-S' chain with one extra site and a decoupled spin $S_{\rm eff}$ of size $S - S'$. The $S' \geqslant 1$ models already exhibit non-generic behaviour before adding the impurity. In particular these integrable periodic models [10, 11], without impurities, do not exhibit the Haldane gap for integer S'. For a discussion see [12]. We shall not consider them further.

A peculiar feature of the integrable impurity model with $S' = 1/2$ and $S \geqslant 1$ is that the effective, partially screened impurity at the critical point has spin $S_{\rm eff} = S - 1/2$ [9], despite the fact that the impurity couples with equal strength to *two* spin-1/2's. This seems contradictory since, if we assume that the critical point corresponds to an infinite antiferromagnetic coupling then we would obtain $S_{\rm eff} = S - 1$. Furthermore, our RG analysis indicates that in any event if $S_{\rm eff} \neq 0$ a stable critical point must correspond to the *open* chain. Our further analysis of the integrable impurity model with $S = 1$, discussed in section 3, indicates that the critical point corresponds to the *periodic* chain with $S_{\rm eff} = S - 1/2 = 1/2$. It is as if the impurity spin 'splits in half', donating an extra $S = 1/2$ spin to the periodic chain and leaving behind a decoupled $s = 1/2$ impurity (see figure 1).

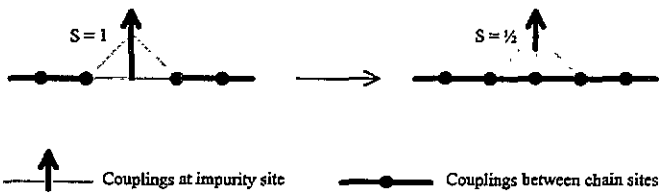

Figure 1. The $S = 1$ impurity effectively 'splits in half', donating an extra $S = 1/2$ impurity to the chain.

We argue below that this corresponds to an unstable critical point which is peculiar to this Hamiltonian. Generic Hamiltonians renormalize to the stable fixed points mentioned above. Thus it appears that the conditions for integrability somehow 'fine-tune' the impurity-model Hamiltonian so that it corresponds to an unstable fixed point. The same phenomenon was found earlier for integrable periodic chains of spin $S' \geqslant 1$ [12].

In the next section we briefly review our RG analysis which shows that the integrable impurity model cannot correspond to any of the known stable fixed points. We then conjecture that it corresponds to the particular unstable fixed point mentioned above. In section 3 we analyse this unstable fixed point. In particular, we find that the RG flow to this fixed point is governed by two marginally irrelevant operators which lead to finite-size corrections which only go away with the inverse logarithm of the chain length. Fortunately, we are able to calculate energy eigenvalues for chain lengths up to 5000 using the Bethe ansatz. This enables us to analyse in detail the logarithmic behaviour and show convincingly that our conjecture is correct. In section 4 we analyse the effect of perturbing the couplings to the impurity. We conjecture a general RG flow and phase diagram and attempt to test it numerically. The non-integrability limits the maximum chain length to about 20. Because of the presence of two marginal operators it is difficult to draw definitive conclusions from these calculations but they seem to be consistent with our conjecture that the integrable impurity model corresponds to an unstable fixed point.

2. Review

The continuum limit of the $S = 1/2$ Heisenberg antiferromagnet, $\boldsymbol{S}_i = (1/2)\boldsymbol{\sigma}_i$, can be written in terms of a free boson, with a particular value of the 'compactification radius' (or Lagrangian normalization) which enforces the $SU(2)$ symmetry. (For a review see [6].) This model is equivalent to the $SU(2)$ Wess–Zumino–Witten model (WZW) with Kac–Moody central charge, $k = 1$. The uniform and staggered magnetization correspond to two different operators. Thus the spin operators, $\boldsymbol{S}_i = (1/2)\boldsymbol{\sigma}_i$, becomes:

$$\boldsymbol{S}_i \approx (\boldsymbol{J}_\mathrm{L} + \boldsymbol{J}_\mathrm{R}) + (-1)^i \mathrm{constant} \cdot \mathrm{tr}\, h\boldsymbol{\sigma}. \tag{2.1}$$

Here $\boldsymbol{J}_\mathrm{L}$ and $\boldsymbol{J}_\mathrm{R}$ are the left and right-moving spin densities or currents and h is an $SU(2)$ matrix field. The current operators have scaling dimension $x = 1$ while h has $x = 1/2$. Using the operator product expansion, it can be shown that,

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \approx \mathrm{constant}(-1)^i\, \mathrm{tr}\, h. \tag{2.2}$$

We now review the effect of local perturbations upon the open and periodic chain fixed points.

The various types of local perturbations of the *periodic* chain corresponding to quantum impurities can all be expressed in terms of $\boldsymbol{J} \equiv \boldsymbol{J}_\mathrm{L} + \boldsymbol{J}_\mathrm{R}$ and h, the former operator being marginal and the latter relevant. In fact, most perturbations generate relevant operators, the only exception being perturbations symmetric under site-parity $\mathcal{P}_S$, i.e. reflection about a site, which *do not* involve an external spin. In this case the parity symmetry ensures that all terms involving $\mathrm{tr}\, h$ cancel. A perturbation which is not invariant under $\mathcal{P}_S$ will generate $\mathrm{tr}\, h$ under a renormalization group transformation. Let us now consider perturbations that *do* involve an external spin. A $\mathcal{P}_S$ invariant coupling, i.e. $\boldsymbol{\sigma}_i \cdot \boldsymbol{S}$, to an external spin $\boldsymbol{S}$ generates the relevant operator $\mathrm{tr}\, h\boldsymbol{\sigma} \cdot \boldsymbol{S}$, as can be seen from (2.1). (Note that $\mathrm{tr}\, h\boldsymbol{\sigma} \cdot \boldsymbol{S}$ is a relevant operator since a decoupled impurity has zero scaling dimension.) For equal Heisenberg coupling of two neighbouring chain-spins to the impurity, symmetric under *link*-parity, i.e. $\boldsymbol{\sigma}_1 \cdot \boldsymbol{S} + \boldsymbol{\sigma}_L \cdot \boldsymbol{S}$, the $\mathrm{tr}\, h\boldsymbol{\sigma} \cdot \boldsymbol{S}$ terms cancel. However, $\mathrm{tr}\, h$ is generated since in this case the site-parity, $\mathcal{P}_S$, is broken. Hence we arrive at the important conclusion that a periodic chain with a decoupled impurity is not a stable fixed point, since relevant operators always will be present.

The situation is different for the *open* chain. In this case the boundary operator formalism identifies left and right-moving operators and the chain-end spins become:

$$\boldsymbol{S}_\pm \propto \boldsymbol{J}_\pm.$$

Here $+$ and $-$ refer to the two sides of the break in the chain and $\boldsymbol{J} \equiv \boldsymbol{J}_\mathrm{L} \equiv \boldsymbol{J}_\mathrm{R}$. Since h doesn't appear as a boundary operator, all perturbations of the open chain are, at most, marginal. A weak coupling of the two sides of the break is irrelevant. A weak coupling to an external spin generates $(\boldsymbol{J}_+ + \boldsymbol{J}_-) \cdot \boldsymbol{S}$, which is analogous to a Kondo coupling. It is marginally relevant for antiferromagnetic coupling and marginally irrelevant for ferromagnetic coupling. Hence the open chain with no decoupled impurity or with an impurity whose coupling flows to zero from the ferromagnetic side are stable fixed points.

Let us now consider the stable fixed points for open spin-chains with *link*-parity symmetric couplings to an external $S = 1$ impurity, a class of models which includes the integrable one. The case of a simple Heisenberg coupling:

$$H_{\text{imp}} = J(\sigma_1 + \sigma_L) \cdot S \tag{2.4}$$

was discussed earlier [6]. If $J < 0$, it renormalizes to zero leaving the open chain with a decoupled $S = 1$ impurity. If $J > 0$ it is marginally relevant and we assume that it renormalizes to ∞. This produces an open chain with two sites removed and no leftover impurity in the low-energy theory.

The excitation spectrum of a long chain of length L contains towers of states with spacings of $O(1/L)$ up to higher-order corrections. This low-energy spectrum, which is a universal property of the fixed point, is reviewed in [6], for periodic and open chains. Some of the first few states are given in table 1 of the present paper. Note that spin chains of even length, L, with periodic or open boundary conditions, have parity even (odd) ground-states for $L/2$ even (odd). To $O(1/L)$, the spectra are identical for $L/2$ even or odd apart from a parity flip for all states. Thus we see that in specifying the various fixed points we must be careful to specify the ground-state parity. The infinite antiferromagnetic J fixed point referred to in the previous paragraph corresponds to a ground-state with reversed parity compared to $J = 0$, since two spins have been effectively removed from the chain to screen the impurity. We will take the original chain length to have $L/2$ even. Thus this screened fixed point has a ground-state with $S_{\text{T}}^P = 0^-$, where S_{T} is the spin of the state and P its parity. We label the renormalization group fixed point corresponding to an open chain with no parity flip as open$^+$; we label the fixed point with the parity flip as open$^-$. The open chain with no parity flip and a leftover decoupled $S = 1$ impurity is labelled open$^+ \times (S = 1)$. Thus a negative J renormalizes to the open$^+ \times (S = 1)$ fixed point and a positive J renormalizes to the open$^-$ fixed point.

Table 1. The low temperature spectra showing *only* the four states $0^+, 0^-, 1^+, 1^-$ for the various fixed points. L is divisible by 4, $x = L(E_n - E_0)/2\pi v$.

x	Integrable model: periodic chain of $L+1$ sites with decoupled spin-1/2 impurity P_I	Open chain of $L-2$ sites with singlet open$^-$	Open chain of L or $L-4$ sites with singlet open$^+$	Open chain of L sites with decoupled spin-1 impurity open$^+ \times (S = 1)$
7/4		0^+	0^-	
5/4		1^-	1^+	0^+
3/4		1^+	1^-	$0^-, 1^-$
1/4	$0^+, 0^-, 1^+, 1^-$	0^-	0^+	1^+

Let us now consider the integrable impurity model of (1.1). The Bethe ansatz results of [9] indicate that the magnetization has Curie form as $T \to 0$ with magnitude corresponding to a decoupled $S = 1/2$ impurity. It is quite easy to see that such a fixed point will not arise in a link-parity invariant model from the type of analysis used above, where it is assumed that all couplings renormalize to ∞ or 0. If a single chain-spin coupled most strongly to the impurity it could partially screen it, leaving an effective $S = 1/2$ impurity. However, with link-parity, this type of analysis always produces changes in the effective spin by integer units. The other possibility is that the $S = 1$ impurity effectively 'splits in half', donating an extra $S = 1/2$ to the chain and leaving behind a decoupled effective $S = 1/2$ impurity (see figure 1). The coupling of the rest of the chain to the 'donated' $S = 1/2$ must 'heal', i.e. renormalize to the same value as in the rest of the chain. Such a healing phenomena was shown to occur for an $S = 1/2$ impurity coupled symmetrically to two neighbouring sites in a chain [6]. However, this does not correspond to a stable fixed point in the present case because of the decoupled $S = 1/2$ impurity. A residual coupling of this to the healed chain is relevant, as discussed above. It generates the operator, $-\lambda' \operatorname{tr} \boldsymbol{h\sigma} \cdot \boldsymbol{S}_{\text{eff}}$, where $\boldsymbol{S}_{\text{eff}}$ is the effective $S = 1/2$ impurity.

We now propose a resolution of this dilemma. Due to the very particular nature of the integrable Hamiltonian (1.1) the relevant coupling, λ', referred to above, vanishes. Of course, if we were to make an infinitesimal change in any of the lattice coupling constants near the impurity, we should expect that this relevant coupling in the fixed point Hamiltonian would generally become non-zero. In the next section we explore, using both RG and finite-size Bethe ansatz analysis, this hypothesis about the integrable impurity model itself. In section 4 we use RG and the modified Lanczos method to study perturbations of the integrable impurity model.

3. The integrable impurity model

We now want to study the integrable impurity model in more detail. As stated above, we hypothesize that it renormalizes to the *unstable* fixed point corresponding to the $S = 1$ impurity breaking up into two $S = 1/2$ spins, one of which is adsorbed into the chain and the other of which decouples (see figure 1). We assume that the chain originally had length L; hence, after adsorbing the extra $S = 1/2$ variable, it has the effective length $l = L + 1$. For this decoupling to occur, the relevant coupling of the extra spin to the chain, discussed in the previous section, must be 'fine-tuned' to zero. The next most important coupling to consider is then the marginal coupling of the impurity to the periodic chain. This can be written:

$$\delta H = -\lambda(l) v (\boldsymbol{J}_{\text{L}} + \boldsymbol{J}_{\text{R}})(0) \cdot \boldsymbol{S}_{\text{eff}} \tag{3.1}$$

where $\boldsymbol{J}_{L,R}(x)$ is the spin-density of left (right)-movers and $\boldsymbol{S}_{\text{eff}}$ is the effective impurity spin assumed to have size $1/2$. v, the spin-wave velocity, plays the role of the velocity of light in the conformal field theory. Its value, $v = \pi/2$, is known exactly from the Bethe ansatz. A positive λ corresponds to a ferromagnetic coupling. The total spin of the left-movers is given by:

$$\boldsymbol{S}_{\text{L}} = \frac{1}{2\pi} \int \mathrm{d}x \, \boldsymbol{J}_{L} \tag{3.2}$$

and similarly for the right-movers. The total spin of the periodic chain (not including $\boldsymbol{S}_{\text{eff}}$) is

$$\boldsymbol{S}_{\text{chain}} = \boldsymbol{S}_{\text{L}} + \boldsymbol{S}_{\text{R}}. \tag{3.3}$$

The β-function for λ is calculated in appendix B of [1]. (See equation (B10.) There a positive λ is antiferromagnetic.) The calculation is identical to that for the Kondo problem and the result is:

$$\mathrm{d}\lambda / \mathrm{d} \ln l = -\lambda^2. \tag{3.4}$$

Although, in that appendix we only have the left-moving part of J, the two parts of the interaction renormalize separately so we get the same β-function. Note that a ferromagnetic coupling is marginally irrelevant. Solving, we obtain the effective coupling constant at scale l in terms of the effective coupling constant at scale l_0 as:

$$\lambda(l) \approx \frac{\lambda(l_0)}{1+\lambda(l_0)\ln(l/l_0)}. \tag{3.5}$$

Thus, if the integrable impurity model is to renormalize to the proposed fixed point, the marginal coupling, λ must be ferromagnetic (i.e. $\lambda > 0$) in addition to the relevant coupling vanishing. There is no particular reason for the marginally irrelevant coupling, λ to be strictly zero, and indeed we shall see that it is not. Such a marginally irrelevant coupling leads to corrections to the asymptotic behaviour which only vanish as $1/\ln l$. Consequently, it becomes difficult to conclude very much about the critical behaviour from finite-size calculations unless exponentially long chains can be studied. Fortunately, this is possible using the Bethe ansatz.

A similar difficulty was already encountered for the periodic $S = 1/2$ chain, without any impurity. In that system there is a 'bulk' marginal operator:

$$\delta H = -g(l)v(8\pi^2/\sqrt{3})\int \mathrm{d}x\, J_{\mathrm{L}}(x)\cdot J_{\mathrm{R}}(x). \tag{3.6}$$

(Recall that dimension *two* bulk operators are marginal, but dimension *one* boundary operators are marginal; the difference arises from the integral over $\mathrm{d}x$ in the former case.) In this case, the renormalized coupling is given by [13]:

$$g(l) = g(l_0)/(1+4\pi g(l_0)\ln(l/l_0)/\sqrt{3}). \tag{3.7}$$

As first pointed out by Cardy [14], and applied to the study of periodic Heisenberg chains in [13], the effect of such marginally irrelevant couplings on the finite-size spectrum can be calculated in perturbation theory in the effective coupling constant.

At a conformally invariant fixed point, excitation energies, take the form [15]:

$$E_n - E_0 = \frac{2\pi v}{l}x_n \tag{3.8}$$

where E_0 is the ground-state energy and the scaling dimensions, x_n, are universal. The x_n's for the lowest energy state of given S_{L}, S_{R} can be written:

$$x_n = (S_{\mathrm{L}})^2 + (S_{\mathrm{R}})^2. \tag{3.9}$$

(see for example [13]). The total spin multiplets are determined by the usual angular momentum addition rules, $|S_{\mathrm{L}} - S_{\mathrm{R}}| \leqslant S_{\mathrm{chain}} \leqslant S_{\mathrm{L}} + S_{\mathrm{R}}$. For an even length chain S_{L} and S_{R} are either both integer or both half-integer; for an odd length chain one of them is integer and one is half-integer.

The ground-state energy takes the form:

$$E_0 = \epsilon_0 l - \frac{\pi v c}{6l} \tag{3.10}$$

where $\epsilon_0 = \ln 2$, the ground-state energy density, is non-universal and the universal $1/l$ correction is proportional to c, the conformal anomaly parameter; $c = 1$ for the $S = 1/2$ chain.

The excitation energies receive corrections in first order perturbation theory in the bulk marginal coupling constant, g [4, 13]:

$$\delta x_n = -\frac{4\pi}{\sqrt{3}} g(l) \boldsymbol{S}_{\mathrm{L}} \cdot \boldsymbol{S}_{\mathrm{R}}. \tag{3.11}$$

Note that this dot product can be determined from S_{L}, S_{R} and S_{chain}:

$$\begin{aligned} \boldsymbol{S}_{\mathrm{L}} \cdot \boldsymbol{S}_{\mathrm{R}} &= \tfrac{1}{2}[(\boldsymbol{S}_{\mathrm{L}} + \boldsymbol{S}_{\mathrm{R}})^2 - \boldsymbol{S}_{\mathrm{L}}^2 - \boldsymbol{S}_{\mathrm{R}}^2] \\ &= \tfrac{1}{2}[S_{\mathrm{chain}}(S_{\mathrm{chain}} + 1) - S_{\mathrm{L}}(S_{\mathrm{L}} + 1) - S_{\mathrm{R}}(S_{\mathrm{R}} + 1)]. \end{aligned} \tag{3.12}$$

The ground-state energy only obtains a correction of third order in $g(l)$ [14, 13]:

$$\delta c = \frac{2\pi g^3(l)}{\sqrt{3}}. \tag{3.13}$$

The integrable impurity model has two marginal coupling constants, $g(l)$ and $\lambda(l)$, producing two sources of logarithmically slow finite-size behaviour. The corrections due to g will be the same as for the periodic chain, given above. We now calculate the corrections due to the marginal boundary coupling constant, λ.

There is a first-order correction to the excitation energies. Since, for $\lambda = 0$, the chain is translationally invariant, for any eigenstate,

$$\langle n|(\boldsymbol{J}_{\mathrm{L}} + \boldsymbol{J}_{\mathrm{R}})(0)|n\rangle = [2\pi/l]\langle n|\boldsymbol{S}_{\mathrm{chain}}|n\rangle. \tag{3.14}$$

The marginal coupling of the impurity to the periodic chain, (3.1), will then give rise to a finite size correction of the scaling dimension of the following form

$$\delta x_n = -\lambda(l) \boldsymbol{S}_{\mathrm{chain}} \cdot \boldsymbol{S}_{\mathrm{eff}}. \tag{3.15}$$

This can be expressed in terms of the observable total spin of the state, S_{T} where $\boldsymbol{S}_{\mathrm{T}} = \boldsymbol{S}_{\mathrm{chain}} + \boldsymbol{S}_{\mathrm{eff}}$, the spin of the periodic chain, S_{chain}, and the impurity spin, $S_{\mathrm{eff}} = 1/2$, giving:

$$\boldsymbol{S}_{\mathrm{chain}} \cdot \boldsymbol{S}_{\mathrm{eff}} = \tfrac{1}{2}[S_{\mathrm{T}}(S_{\mathrm{T}} + 1) - S_{\mathrm{chain}}(S_{\mathrm{chain}} + 1) - 3/4]. \tag{3.16}$$

Combining the various terms we obtain

$$E_n - E_{1/2} = \frac{2\pi v}{l}\left[S_{\mathrm{L}}^2 + S_{\mathrm{R}}^2 - \frac{4\pi}{\sqrt{3}} g(l) \boldsymbol{S}_{\mathrm{L}} \cdot \boldsymbol{S}_{\mathrm{R}} - \lambda(l) \boldsymbol{S}_{\mathrm{chain}} \cdot \boldsymbol{S}_{\mathrm{eff}}\right] \tag{3.17}$$

where the effective length, l, for the integrable impurity model is $l = L + 1$.

The correction to the energy of the ground state, which has $S_{\mathrm{L}} = S_{\mathrm{R}} = S_{\mathrm{chain}} = 0$, $S_{\mathrm{T}} = 1/2$, vanishes to first order in λ, so let us consider next order. We can express the second-order correction in terms of the expansion of the partition function in powers of λ in the zero-temperature limit. This gives:

$$Z = Z_0\left[1 + \tfrac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau_1\, \mathrm{d}\tau_2\, \langle \delta H(\tau_1) \delta H(\tau_2)\rangle + \cdots\right]. \tag{3.18}$$

Thus the correction to the ground-state energy is:

$$\delta E_0 = -\tfrac{1}{2}(v\lambda)^2 \int_{-\infty}^{\infty} \mathrm{d}\tau \, \langle 0|(J_\mathrm{L}+J_\mathrm{R})(0,0)\cdot S_\mathrm{eff}(0)(J_\mathrm{L}+J_\mathrm{R})(\tau,0)\cdot S_\mathrm{eff}(\tau)0\rangle. \tag{3.19}$$

In lowest-order perturbation theory:

$$\langle 0|S^a_\mathrm{eff}(0)S^b_\mathrm{eff}(\tau)|0\rangle = \tfrac{1}{3}\delta^{ab}S^2_\mathrm{eff} = \tfrac{1}{3}\delta^{ab}s(s+1) = \tfrac{1}{4}\delta^{ab}. \tag{3.20}$$

We also need:

$$\langle 0|J^a_\mathrm{L}(\tau)J^b_\mathrm{L}(0)|0\rangle = \delta^{ab}/2(v\tau)^2 \tag{3.21}$$

and the same for J_R. (Left and right are uncorrelated. See [1] for the normalization.) This is just the free fermion current Green's function. This is the result for an infinite system. To get the result for a finite system we make a conformal transformation to map the infinite plane onto the cylinder of circumference l, or else just work out explicitly the free fermion current Green's function with appropriate boundary conditions. The result is:

$$\langle 0|J^a_\mathrm{L}(\tau)J^b_\mathrm{L}(0)|0\rangle = \delta^{ab}\frac{1}{2[(l/\pi)\sinh(\pi v\tau/l)]^2}. \tag{3.22}$$

Note that the τ integral in (3.18) diverges as $\tau \to 0$. This is an ultraviolet divergence which would be cut off by the lattice spacing of the spin chain. It is simplest just to put in a cut off on the τ integral, $|\tau| > \tau_0$. To evaluate the integral we change variables to $u = \tanh(\pi v\tau/l)$, giving:

$$\delta E_0 = -\tfrac{3}{4}\lambda^2 v\frac{\pi}{l}\int_{u_0}^{1} \mathrm{d}u/u^2 \tag{3.23}$$

where $u_0 \approx \pi v\tau_0/l$. (We assume $l \gg \tau_0$.) Thus

$$\begin{aligned}\delta E_0 &= -\tfrac{3}{4}\lambda^2 v\frac{\pi}{l}(1/u_0 - 1)\\ &= -3\lambda^2/4\tau_0 + 3\lambda^2 v(\pi/4l).\end{aligned} \tag{3.24}$$

Note that the first, cut-off dependent term, is a non-universal contribution to the l-independent part of E_0. The second is a correction to c:

$$\delta c = -\tfrac{9}{2}\lambda^2(l). \tag{3.25}$$

The universal ground-state energy correction is second order in λ but third order in g; we find that the λ correction is much larger. Assembling the various terms the ground-state energy takes the form:

$$E_{1/2} - \varepsilon_0 L - \varepsilon_1 = -\frac{2\pi v}{12l}\left[1 + \frac{[2\pi g(l)]^3}{\sqrt{3}} - \tfrac{9}{2}\lambda^2(l)\right] \tag{3.26}$$

where we should use $l = L + 1$ for the integrable impurity model. Here $\varepsilon_0 = \ln 2$, and from the work of Schlottmann [9] $\varepsilon_1 = \frac{1}{2}(\psi(3/4) - \psi(5/4)) \simeq -0.429\,203\,673\,3$, where ψ is the digamma function.

The ground state, with $S_{\mathrm{T}} = 1/2$, occurs for L odd corresponding to the effective length, $l = L + 1$, being even. All states occurring for even L are regarded as excited states. In applying (3.17), the values of $g(l)$ and $\lambda(l)$ are expected to interpolate smoothly between even and odd l. In table 4, we give all the relevant quantum numbers for the first few lowest energy states. Note that the states with half-integer S_{chain} all come in pairs of opposite parity, obtained by interchanging the quantum numbers S_{L} and S_{R}. These pairs are degenerate including $\mathrm{O}(\lambda)$ corrections. Presumably they are, for more general models, split by corrections of higher order in irrelevant operators. However, as we shall see, for the integrable impurity model they remain exactly degenerate.

In what follows, we test these formulae in two different ways. One way is to confirm that all energy levels that we consider are given by these formulae with the same values for $g(l)$ and $\lambda(l)$ for a given length $l = L+1$. We expect small discrepancies to occur because of corrections in higher orders of perturbation theory; however, these should become smaller at larger l. Secondly, the functions $g(l)$ and $\lambda(l)$ should be given by the lowest-order β-function results, (3.5) and (3.7) for sufficiently large l.

Following Andrei and Johannesson [7] the Bethe ansatz equations, for the integrable Hamiltonian of (1.1), are

$$\left(\frac{\Lambda_k + \mathrm{i}\frac{1}{2}}{\Lambda_k - \mathrm{i}\frac{1}{2}}\right)^L \left(\frac{\Lambda_k + \mathrm{i}}{\Lambda_k - \mathrm{i}}\right) = -\prod_{l=1}^{M} \frac{\Lambda_k - \Lambda_l + \mathrm{i}}{\Lambda_k - \Lambda_l - \mathrm{i}} \tag{3.27}$$

where L is the number of $S = 1/2$'s. The number of roots, M determines the total S^z component through the relation $S^z = \frac{1}{2}L + 1 - M$. In terms of the solutions, Λ_k, to the Bethe ansatz equations (3.27) the energy is given by

$$E = -\sum_{k=1}^{M} \frac{\frac{1}{2}}{\Lambda_k^2 + (\frac{1}{2})^2}. \tag{3.28}$$

One should note that the energy, E_{H}, of the Hamiltonian (1.1) is related to E by $E_{\mathrm{H}} = E + \frac{1}{4}L + \frac{2}{9}$.

The Bethe ansatz equations are solved numerically by first making the assumption that the solutions occur in strings of length n.

$$\Lambda_j^{n,\alpha} = \Lambda_j^n + \mathrm{i}(n + 1 - 2\alpha)/2 \qquad \alpha = 1, \ldots, n \tag{3.29}$$

and then solving (3.27) for the centres of the strings, Λ_j^n. If ν_n is the number of strings of length n then we must have

$$M = \sum_n n\nu_n. \tag{3.30}$$

The string assumption is then relaxed and the full Bethe ansatz equations are solved by a Newton–Raphson method using the string solution as the starting point.

For chains of even length, $L + 1$, corresponding to an *odd* number, L, of sites with $S = 1/2$ and one spin $S = 1$, we determine the three lowest-lying levels, $E_{1/2}$, $E_{3/2}$ and $E^*_{1/2}$. Here the index refers to the total spin, S_{T}, of the state. The ground-state $E_{1/2}$ corresponds to a solution with $(L + 1)/2$ real roots and no strings, $E_{3/2}$ is a solution with $(L - 1)/2$ real roots and $E^*_{1/2}$ has $(L - 3)/2$ real roots plus a 2-string at $x \pm \mathrm{i}(\pi/2 + \delta)$ where δ is a small positive number quickly approaching zero for long chains, and x is non-zero.

Table 2. Spectrum of the integrable impurity model for *even* chains, corresponding to an odd number, L, of sites with $S = 1/2$ plus one spin $S = 1$. The levels shown are the ground state, $E_{1/2}$, which has $S = 1/2$, the first excited state, $E_{3/2}$, which has $S = 3/2$, and the second excited state, $E^*_{1/2}$, which has $S = 1/2$.

L	$-E_{1/2}$	$-E_{3/2}$	$-E^*_{1/2}$
3	2.666 666 666 667	2.000 000 000 000	0.833 333 333 333
5	4.000 000 000 000	3.535 183 758 488	2.788 431 731 592
7	5.360 920 843 433	5.000 000 000 000	4.473 627 449 978
9	6.732 050 807 569	6.435 509 583 680	6.035 934 151 803
11	8.108 179 626 193	7.855 772 506 636	7.536 851 526 445
13	9.487 154 267 776	9.267 023 613 165	9.003 326 289 075
15	10.867 912 224 042	10.672 479 361 373	10.448 698 007 398
17	12.249 865 197 376	12.073 976 382 835	11.880 255 773 559
19	13.632 659 805 114	13.472 643 412 759	13.302 298 857 367
21	15.016 070 414 566	14.869 214 052 794	14.717 519 700 013
99	69.058 063 860 390	69.021 685 474 014	68.996 582 070 614
199	138.369 221 288 792	138.350 334 224 364	138.339 077 391 494
399	276.996 826 009 204	276.987 093 406 252	276.981 995 627 127
599	415.625 640 252 833	415.619 054 638 227	415.615 834 877 143
799	554.254 762 484 295	554.249 776 039 106	554.247 448 415 855
999	692.884 009 113 116	692.879 992 507 487	692.878 181 269 8
2047	1419.301 863 049 853	1419.299 863 460 628	—
4999	3465.472 116 743 763	3465.471 281 523 977	—

Table 3. Spectrum of the integrable impurity model for *odd* chains, corresponding to an even number, L, of sites with $S = 1/2$ plus one spin $S = 1$. The levels shown are the ground state, E_1, which has $S = 1$, and the second excited state, E_2, which has $S = 2$.

L	$-E_1$	$-E_2$
2	1.333 333 333 333	0.000 000 000 000
4	2.951 367 322 083	1.767 591 879 244
6	4.413 722 666 901	3.489 392 593 998
8	5.839 581 489 564	5.090 273 141 761
10	7.250 399 759 403	6.621 632 325 853
12	8.653 468 913 494	8.111 911 768 408
14	10.051 996 142 025	9.576 268 507 776
16	11.447 623 604 652	11.023 300 473 744
18	12.841 282 703 621	12.458 202 998 467
20	14.233 542 424 308	13.884 288 605 831
100	69.731 013 913 337	69.651 755 717 692
200	139.052 006 805 828	139.011 131 675 689
400	277.684 686 429 578	277.663 763 091 977
600	416.315 227 987 524	416.301 121 655 718
800	554.945 223 280 210	554.934 568 453 894
1000	693.574 997 489 704	693.566 430 520 955
2046	1418.607 647 701 090	1418.603 401 388 401

The results for these three levels are given in table 2. For chains of odd length, $L + 1$, corresponding to an *even* number, L, of sites with $S = 1/2$ plus one site with spin $S = 1$, we determine the two levels E_1 and E_2. E_1, the lowest lying state, is a solution of the Bethe ansatz equations with $L/2$ real roots. We were not able to obtain the first excited state, E_0, by the Bethe ansatz scheme. The next excited level, E_2, has $L/2 - 1$ real roots. The results for E_1 and E_2 are summarized in table 3.

Table 4. The quantum numbers S_L, S_R, S_{chain}, $S_L \cdot S_R$, $S_{chain} \cdot S_{eff}$, and x for the five levels, describing the integrable impurity model.

S_T^P	S_L	S_R	S_{chain}	$S_L \cdot S_R$	$S_{chain} \cdot S_{eff}$	x
$L+1$ odd						
$2^+, 2^-$	1	1/2	3/2	1/2	3/4	5/4
$0^+, 0^-$	1/2	0	1/2	0	−3/4	1/4
$1^+, 1^-$	1/2	0	1/2	0	1/4	1/4
$L+1$ even						
$1/2^{*+}$	1/2	1/2	0	−3/4	0	1/2
$1/2^{*-}$	1/2	1/2	1	1/4	−1	1/2
$3/2^-$	1/2	1/2	1	1/4	1/2	1/2
$1/2^+$	0	0	0	0	0	0

These states exhibit some remarkable degeneracies, for finite L. Equation (3.27) is invariant under the operation, $\{\Lambda_k\} \to \{-\Lambda_k\}$. Thus, in cases where the set of roots is not symmetric about 0, a pair of degenerate solutions is obtained, if we assume that the corresponding wavefunctions are linearly independent as can be verified for short chains. This is the case for all solutions discussed above with even L and also for $(1/2)^*$. The even L degeneracies can be understood from the picture of the RG fixed point corresponding to a periodic chain of $(L+1)$ $S = 1/2$ and a decoupled $S = 1/2$. The periodic odd-length chain has a large exact degeneracy for finite L. This follows from the fact that the ground-state does not have zero momentum. Instead it consists of two degenerate doublets, $(1/2)^{\pm}$ with momentum $\pm k_0$. As $L \to \infty$, we expect $k_0 \to \pi/2$. By forming linear combinations of these states we can form positive and negative parity eigenstates. All low-lying states have momentum close to $\pm\pi/2$ and consequently also come in parity doublets. In the conformal field theory picture, the parity doubling arises from the fact that the periodic chain of odd length, $L+1$ has S_L integer and S_R half-integer or vice versa. The corrections to the excitation energies of first order in g and λ (3.17) do not lift the degeneracy. This must be true to all orders in g and all other irrelevant bulk operators for the periodic chain. On the other hand, we expect that higher-order corrections in irrelevant boundary operators will, in general, lift the degeneracy since momentum is not, in general, a well defined quantum number for the impurity system. Remarkably, this does not happen for the integrable impurity model and the degeneracy remains exact. Even more surprising is the degeneracy for odd L. In this case the corresponding periodic chain has even length, $L+1$ and does not exhibit any exact finite-length degeneracies. Nonetheless, such a degeneracy occurs for the $(1/2)^{\pm *}$ states. We see from table 4 that this occurs via a cancellation of the $O(g)$ and $O(\lambda)$ marginal corrections. At large l, using $\lambda(l) \to 1/\ln(l)$, $g(l) \to \sqrt{3}/4\pi \ln(l)$ the correction to x_n becomes:

$$\delta x_n = -[S_L \cdot S_R + S_{chain} \cdot S_{eff}]/\ln l. \tag{3.31}$$

$[S_L \cdot S_R + S_{chain} \cdot S_{eff}]$ has the value $-3/4$ for both the $(1/2)^{*+}$ and $(1/2)^{*-}$ state. The splitting of these levels by the marginal bulk operator is cancelled by the splitting due to the marginal boundary operator! Furthermore, this cancellation must be exact to all orders in irrelevant bulk and boundary operators. This suggests the existence of some sort of hidden symmetry in the integrable impurity model reminiscent of the Yangian symmetry discussed recently for the $1/r^2$ periodic Heisenberg chain [16].

We can now try to extract the coupling constant, $\lambda(l)$ defined in (3.1), as determined from the five levels, $E_{1/2}$, $E_{3/2}$, $E^{*-}_{1/2}$, E_1 and E_2. The bulk marginal coupling constant,

$g(l)$, has already been determined from finite-size analysis of long *periodic* chains without the impurity [13]. We shall use this as input and determine the boundary marginal coupling, $\lambda(l)$ from our data on the integrable impurity model. Thus the only free parameter is $\lambda(l)$. Note that (1/2) is the ground state so we fit its energy to (3.26). The other four are excited states so we fit their excitation energies by (3.17). The different estimates of $\lambda(l)$ obtained from the different energy levels are shown in figure 2. Notice, first of all that λ is positive, corresponding to a ferromagnetic, marginally irrelevant coupling of S_{eff} to the chain. As expected the different estimates of $\lambda(l)$ are all approximately the same. As l increases, the estimated couplings approach each other and get smaller. This is shown in the inset in figure 2 where $(\lambda_i - \lambda_{\text{av}})/\lambda_{\text{av}}$ is plotted as a function of $1/\log(l)$. Here λ_{av} is the average of the five couplings. The λ_is should only differ by amounts of $O(\lambda^2)$ when λ is small and we therefore expect $(\lambda_i - \lambda_{\text{av}})/\lambda_{\text{av}}$ to converge to zero linearly in $1/\log(l)$ for large enough l. This appears consistent with the results shown in the inset in figure 2.

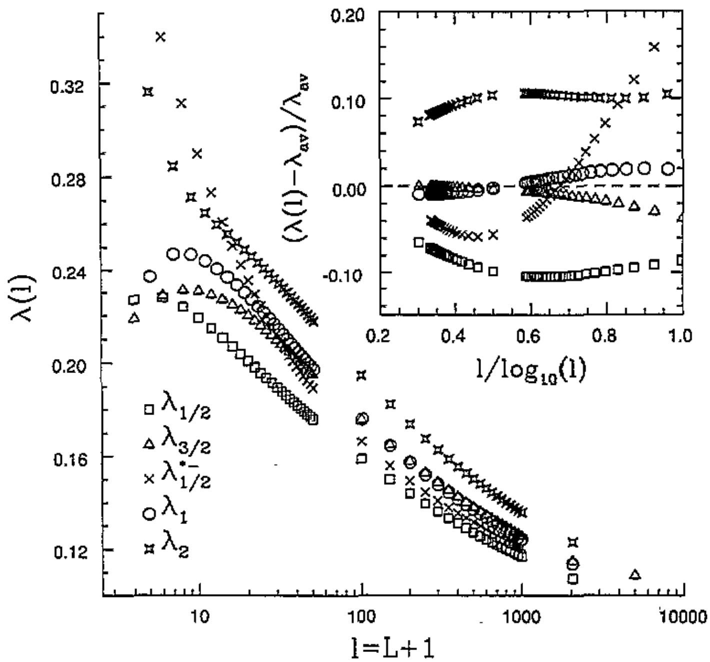

Figure 2. The coupling constant, λ_i, for the five levels, $E_{1/2}$, $E_{3/2}$, $E^{*-}_{1/2}$, E_1 and E_2, as a function of the effective chain length, $l = L + 1$. The inset shows $(\lambda_i - \lambda_{\text{av}})/\lambda_{\text{av}}$, where λ_{av} is the average of the five couplings. We expect this quantity to converge to zero linearly in $1/\log(l)$.

We compare $\lambda(l)$ to the one-loop β-function result (3.5), λ_{rg}, in figure 3. It is seen that the first-order β-function result is valid for chains longer than $l \sim 100$, indicating that our perturbative results should be meaningful for chains of this length or longer. A similar plot for the other coupling g is shown in figure 4. Again we see that the one-loop β function gives good results for chains longer than a few hundred. As shown in table 4 the excited state $(1/2)^{*+}$ does not receive a correction to its excitation energy of first order in λ. We can therefore use it to extract an estimate of $g(l)$ independent of the results from [13]. This estimate, $g_{1/2}(l)$, is also shown in figure 4. It compares nicely to the β-function

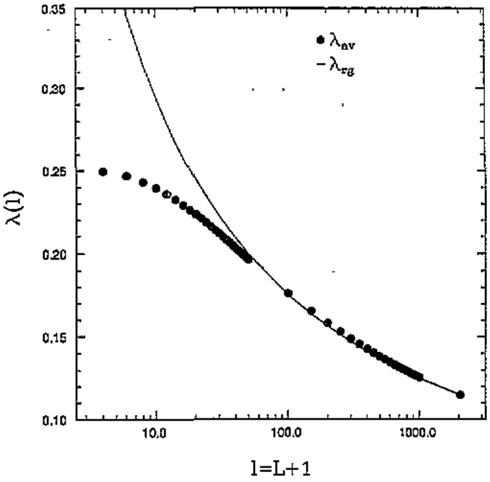

Figure 3. The average of the five coupling constants, λ_{av}, $\lambda = (\lambda_{1/2} + \lambda_{3/2} + \lambda^{+-}_{1/2} + \lambda_1 + \lambda_2)/5$, as a function of the effective length, $l = L + 1$, compared to the one-loop renormalization group prediction, $\lambda_{\mathrm{rg}} = \lambda_{\mathrm{av}}(l_0)/(1 + \lambda_{\mathrm{av}}(l_0)\ln(l/l_0))$. In this plot we have used $l_0 = 1000$.

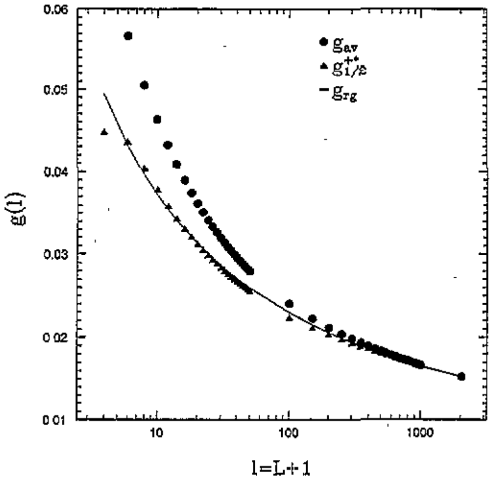

Figure 4. The coupling $g^{+*}_{1/2}$ and the average of the coupling, g_{av}, from [13], as a function of the effective chain length, $l = L + 1$, compared to the one-loop renormalization group prediction, $g_{\mathrm{rg}} = g_{\mathrm{av}}(l_0)/(1 + 4\pi g_{\mathrm{av}}(l_0)\ln(l/l_0)/\sqrt{3})$. In this plot we have used $l_0 = 1000$.

results as well as to the results obtained for the pure periodic $S = 1/2$ chain in [13]. (The corresponding plot in [13] contained a numerical error in the calculation of g_{rg}.)

From the above results we conclude that the spectrum of the integrable impurity model indeed asymptotically becomes that of a periodic chain with $L+1$ spin-1/2's and a decoupled $S_{\mathrm{eff}} = 1/2$. The impurity spin $S = 1$ has effectively split in half. The spectrum corresponds to column 1 in table 1.

4. General Hamiltonians

In this section, we consider the effects of perturbing the integrable impurity Hamiltonian H_{Int} (1.1) away from its integrable form. A general phase diagram is hypothesized and is tested using the modified Lanczos method for general Hamiltonians on chains with $L \leqslant 20$. To be concrete, we consider the following two-parameter set of Hamiltonians:

$$
\begin{aligned}
H &= \frac{1}{4}\sum_{i=1}^{L-1} \sigma_i \cdot \sigma_{i+1} + H_{\mathrm{I}} \\
H_{\mathrm{I}} &= \frac{2J_1}{9}\left[(\sigma_1 + \sigma_L)\cdot S + \tfrac{1}{2}\{\sigma_1 \cdot S, \sigma_L \cdot S\} - \tfrac{7}{8}\sigma_1 \cdot \sigma_L\right] + \frac{J_2}{2}(\sigma_1 + \sigma_L)\cdot S.
\end{aligned}
\tag{4.1}
$$

Here S is the $S = 1$ impurity. $J_1 = 1$, $J_2 = 0$ is the integrable impurity model, and $J_1 = 0$ corresponds to the models discussed in [6]. $J_1 = J_2 = 0$ is the simple open chain with a decoupled $S = 1$ impurity. By combining our understanding of the phase diagram near $|J_i| = 0$, $|J_i| \to \infty$ and the integrable impurity model, we hypothesize a general phase diagram.

The vicinity of $|J_i| = 0$ can be readily analysed. Near the open chain fixed point the terms $\{\sigma_1 \cdot S, \sigma_L \cdot S\}$ and $\sigma_1 \cdot \sigma_L$ in (4.1) contain a product of *both* chain-end spins σ_1 and σ_L. In the continuum limit they correspond to a dimension 2 irrelevant operator containing the product of J_+ and J_-. Thus for small J_i we may approximate the impurity part of the Hamiltonian, H_1, by $(2J_1/9 + J_2/2)(\sigma_0 + \sigma_L) \cdot S$. This is marginally irrelevant for $(J_2 + 4J_1/9) < 0$. Thus, for $(J_2 + 4J_1/9) < 0$, the system renormalizes to the fixed point consisting of the open chain with a decoupled $S = 1$ impurity which we denote by open$^+ \times (S = 1)$. For $(J_2 + 4J_1/9) > 0$ the coupling is *antiferromagnetic* and therefore marginally relevant. We expect it to renormalize to ∞, screening the impurity and effectively removing two sites from the chain. This produces a parity flip, giving the open$^-$ fixed point. (Recall from section 2 that the removal of two spins from the open chain by the screening process reverses the parity.) This transition is ∞-order since it is driven by a marginal operator, i.e. the cross-over length scale diverges exponentially as $(2J_1/9 + J_2/2) \to 0$ from positive values.

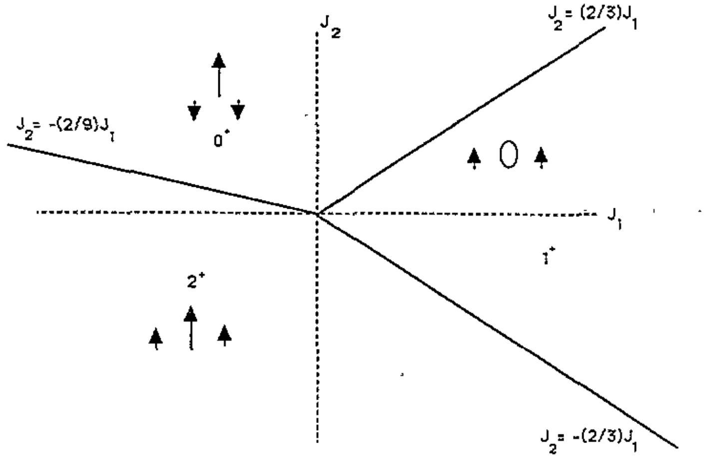

Figure 5. Schematic drawing of the ground-state wavefunctions for the three-spin system depending on J_i. '0' denotes the $S^z = 0$ state of the $S = 1$ impurity.

Let us next consider what happens in the limit $|J_i| \to \infty$. In this limit we must find the ground state of the three-spin system, S, σ_1, σ_L, of H_I. Depending on the J_i's, the ground state has spin and parity 0^+, 1^+ or 2^+. These wavefunctions are depicted schematically in figure 5, as are the regions of stability of the three states. The 0^+ case leads directly to a stable fixed point when we include the relatively weak coupling of these three spins to the rest of the chain. These couplings are irrelevant, leaving the open chain fixed point open$^-$. The 2^+ impurity state, however, is unstable because the effective $S = 2$ impurity is coupled antiferromagnetically to the chain. Assuming this coupling flows to ∞, the impurity is partially screened, leaving an effective $S = 1$ impurity with a *ferromagnetic* coupling to the rest of the chain. Hence, it will renormalize to 0. Since four sites are involved in producing the effective $S = 1$ decoupled impurity, there is no parity flip. Thus we obtain the open$^+ \times (S = 1)$ phase. Of special interest is the 1^+ ground state for the three-spin complex. σ_1 and σ_L form an $S = 1$ spin, symmetric under interchanging these two spins. This then couples to the $S = 1$ impurity to form a state of total spin 1. Note that neither the minimal spin (0) nor the maximal spin (2) occurs. The biquadratic term in H_I, involving the anticommutator, is necessary to assure that this happens. Thus we begin to see how the integrable impurity model can have different behaviour than the simpler one discussed above, with $J_1 = 0$. The 1^+ state of the three-spin cluster does not correspond to a stable fixed point since the rest of the chain is coupled antiferromagnetically to the effective $S = 1$ impurity, and such a coupling is marginally relevant. We expect this coupling to the next two spins in the chain, σ_2 and σ_{L-1} to also renormalize to ∞, screening the effective impurity and leading to an open chain fixed point with no leftover impurity spin. In this case, four chain-spins are involved in screening the impurity in a parity-symmetric way, so that the stable fixed point is open$^+$.

For large $|J_i|$, we expect the above three different stable phases to occur, with the phase boundaries asymptotically approaching those of the three-spin system, as drawn in figure 6. Note that the open$^+ \times (S = 1)$ phase is equivalent to $J_i = 0$, an open chain with a decoupled $S = 1$ impurity; we may think of this entire phase as renormalizing to the origin. The open$^+$ and open$^-$ phases, however, are characterized by impurity couplings renormalizing to ∞.

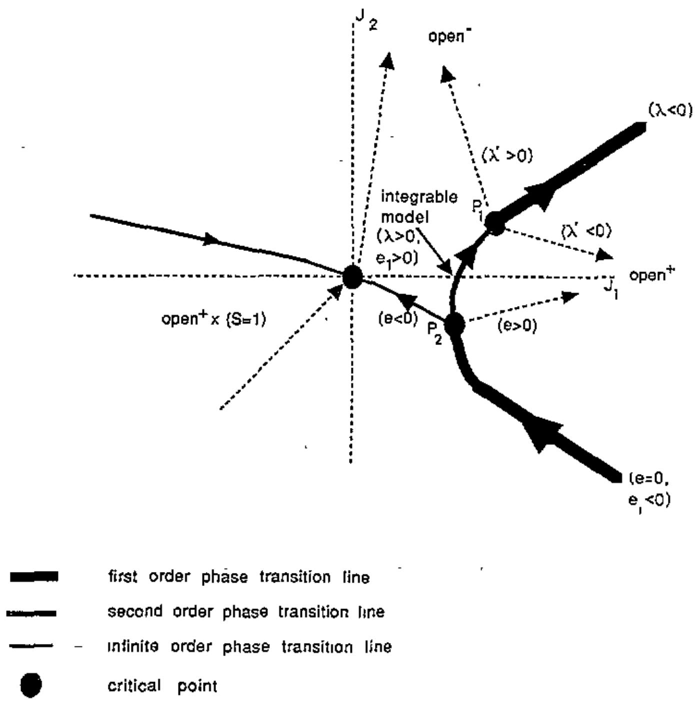

Figure 6. The conjectured phase diagram for the general Hamiltonian (4.1) in the parameter space J_1, J_2. The couplings λ, λ' are defined in the vicinity of the multi-critical point P_1 in (4.2). The couplings e, e_i are defined in the vicinity of the multi-critical fixed point, P_2, in (4.3).

We have established, in the previous section, that the integrable impurity model renormalizes to a fixed point in which the $S = 1$ impurity effectively splits in half, one extra $S = 1/2$ being absorbed by the chain and the other decoupling. This can only occur if no relevant operator connects the periodic chain to the decoupled $S = 1/2$ spin. We now analyse the effect of small perturbations around the integrable impurity model by considering the periodic chain with both marginal and relevant couplings to the effective

$S = 1/2$ impurity, i.e. we consider the continuum limit Hamiltonian consisting of the $k = 1$ WZW model with two local perturbations:

$$\delta\mathcal{H} = -[\lambda' \operatorname{tr} h\sigma + \lambda(J_L + J_R)] \cdot S_{\text{eff}}. \tag{4.2}$$

The integrable impurity model has $\lambda' = 0$, $\lambda > 0$; i.e. the relevant coupling vanishes and the marginal one has the irrelevant sign. An infinitesimal perturbation of the integrable impurity model will, in general, produce a non-zero λ'. The resulting behaviour was discussed in [6], in the context of a simple coupling of an $S = 1/2$ impurity to a single site in a periodic chain. We expect that λ' will renormalize to $\pm\infty$ beginning from an infinitesimal positive (or negative) value. The negative case, corresponding to an antiferromagnetic coupling, leads to screening of S_{eff} by a single site in the chain. The stable fixed point is an open chain with one site removed, open$^+$. For $\lambda' > 0$, the ferromagnetic case, S_{eff} and the site to which it is coupled form an effective $S = 1$ impurity. However, this is not a stable fixed point. The $S = 1$ effective impurity is coupled antiferromagnetically to two neighbouring spins. We expect this coupling to renormalize to ∞, screening the effective impurity. Once again the stable fixed point is an open chain. However, in this case, *three* chain spins are involved in the screening process and get removed from the effective open chain at the stable fixed point. As discussed in section 2, the parity of all low-energy states is flipped relative to the case where a single chain-spin is removed. Thus the stable fixed point in this case is the open$^-$. We see that the unstable critical point, $\lambda' = \lambda = 0$, to which the integrable impurity model renormalizes separates the stable open$^+$ and open$^-$ phases.

We now turn to a discussion of the order of the phase transition separating the open$^+$ and open$^-$ phases. We expect that a second-order critical line will exist for a finite range of positive λ with $\lambda' = 0$ governed by the $\lambda = \lambda' = 0$ critical point. On the other hand, if the marginal coupling $\lambda < 0$, then it is relevant and renormalizes to large values. In this case, the simplest assumption is that $\lambda \to -\infty$; otherwise we would be forced to postulate another non-trivial critical point. In general, when impurity couplings renormalize to ∞ we expect a first-order phase transition. The reason is that we can then ignore any couplings of the impurity complex to the rest of the chain. In this particular case we can consider only the $S = 1/2$ impurity and three chain spins. This cluster of four $S = 1/2$'s has a 0^+ or 0^- ground state depending on the various couplings. The phase transition in this limit is a simple level-crossing in the four-spin system and is therefore first order. The critical point, P_1, at $\lambda = \lambda' = 0$ is on the phase boundary between open$^+$ and open$^-$ phases and separates the second- from first-order transition lines. The integrable impurity model, which was shown in the last section to have a non-zero positive λ, lies on the second-order part of the phase boundary.

Now we attempt to combine our information about the small J_i, large J_i regions and the vicinity of the integrable point. Our large J_i analysis tells us that there are three stable phases, open$^-$, open$^+$ and open$^+ \times (S = 1)$. Our analysis of the vicinity of the integrable impurity model tells us that it should be on the open$^-$–open$^+$ phase boundary. It renormalizes to a critical point, P_1 in figure 6 where this transition changes from first to second order.

The open$^-$ phase occurs when we *increase* J_2 from P_1. This is to be expected because J_2 corresponds to a coupling of S_{eff} to the two nearest neighbours, σ_1, σ_L, not to the adjacent spin σ_0, as shown in figure 7. Antiferromagnetic J_2, i.e. $\lambda' > 0$, leads to a screening of S_{eff} by σ_0, σ_1 and σ_L. The removal of σ_0, σ_1 and σ_L from the open chain leaves a chain with $L - 2$ sites and thereby implies a parity flip. In figure 8 we show a Lanczos calculation

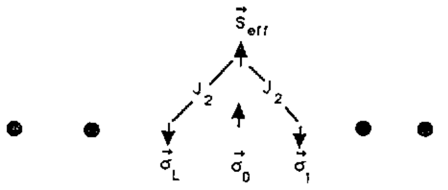

Figure 7. S_{eff} couples with strength J_2 to the two nearest-neighbour spins, σ_1 and σ_L. Antiferromagnetic J_2 leads to screening of S_{eff} by three chain spins and hence to the open$^-$ phase.

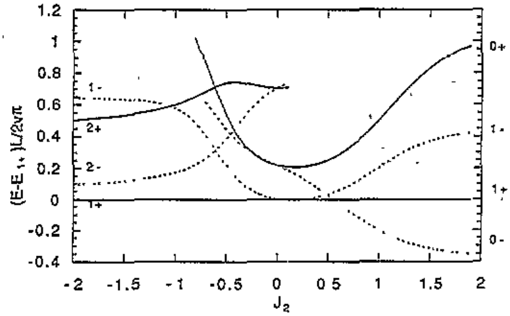

Figure 8. Scaled energy gaps, $L(E - E_{1^+})/2\pi v$, as a function of J_2 ($J_1 = 1$, $L = 20$).

of some low-lying states for length 20, as a function of J_2. The open$^-$ spectrum shown in table 1 occurs for positive J_2. The Lanczos results are discussed in more detail below.

We see that there must be another multi-critical point in the phase diagram where all three stable phases meet, P_2 in figure 6. This point is presumably not at the origin since there is only one marginal operator in the vicinity of the origin, $(2J_1/9+J_2/2)(\sigma_0+\sigma_L)\cdot S$, as discussed above, so we only expect two phases to meet at that point. We hypothesize that this higher multi-critical point corresponds to an open chain with *two* $S = 1/2$ effective impurities, S_1 and S_2, decoupled from the chain and from each other. i.e. the original $S = 1$ impurity effectively breaks up into two $S = 1/2$ impurities, with everything decoupled at the multi-critical point. There is one relevant coupling and two marginal ones at this critical point. We write these, in the lattice model as:

$$\delta\mathcal{H} = eS_1 \cdot S_2 + e_1 S_1 \cdot (\sigma_1 + \sigma_L) + e_2 S_2 \cdot (\sigma_1 + \sigma_L) \tag{4.3}$$

(see figure 9.) We now analyse the phase diagram for this model. Since the impurity spins have zero scaling dimension, the coupling e is highly relevant. Assuming that a non-zero e renormalizes to $\pm\infty$, the two impurities lock into a singlet leaving the open chain fixed point, open$^+$, for $e > 0$. For $e < 0$ they lock into an effective $S = 1$ impurity. If both couplings $e_i < 0$ (ferromagnetic), this $S = 1$ impurity decouples, giving the open$^+ \times (S = 1)$ phase. On the other hand if at least one of the couplings e_i is antiferromagnetic, then the effective $S = 1$ impurity is screened, giving the open$^-$ phase. The open$^+ \times (S = 1) -$open$^-$ phase transition is equivalent to the one discussed in the second paragraph of this section. It is therefore of ∞-order. Note that the open$^+$ $\times$ $(S = 1)$ to open$^+$ phase transition is controlled by the multi-critical point, P_2 at $e = e_i = 0$. This transition is governed by the relevant coupling constant e, which only involves the two impurities and not the rest of the chain. Thus it corresponds to a simple level-crossing in this two-spin system and so should be first order. We hypothesize that, as we move along the critical line, where $e = 0$, one of the marginal couplings, say e_1, changes sign at the multi-critical point, while the other remains ferromagnetic. The transition between open$^-$ and open$^+$ phases, for $e_1 > 0$, is governed by the behaviour at e_1 of O(1). We know that a single $S = 1/2$ impurity with such a coupling to an open chain will get absorbed by the chain, i.e. the defect heals and the fixed point is the periodic chain with an extra spin. Thus it is plausible that this phase boundary is second-order and renormalizes to a periodic chain with a single decoupled

$S = 1/2$ impurity. Note that the continuation of the open$^+ \times (S = 1)$–open$^+$ phase boundary is the open$^-$–open$^+$ phase boundary, but the order of the transition changes from first to second, as drawn in figure 6. This follows from the fact that both phase boundaries are governed by the vanishing of the relevant coupling constant, e. The system renormalizes to P_1 by one of the impurities being absorbed into the chain. It renormalizes to the origin by the two impurities locking into a decoupled $S = 1$ impurity.

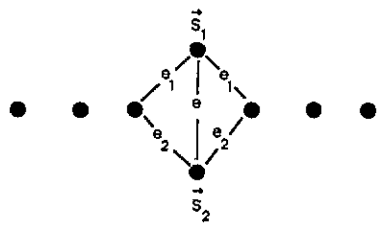

Figure 9. The unstable fixed point P_2 occurring in the phase diagram, figure 6.

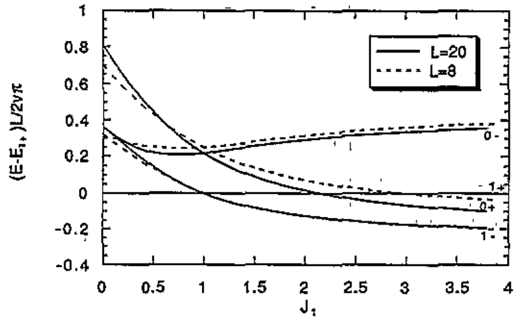

Figure 10. Scaled energy gaps, $L(E - E_{1^+})/2\pi v$, as a function of J_1 ($J_2 = 0$, $L = 8, 20$).

Altogether there are five different critical points; three occurring at finite coupling, P_1, P_2, open$^+ \times (S = 1)$ and two at infinity, open$^+$, open$^-$, as shown in figure 6. Various sections of the transition lines are first, second or infinite order. The detailed shape of the phase boundaries depicted schematically in figure 6 is not known. What is known is (i) the asymptotic slope of the three phase boundaries at $|J_i| \to \infty$, (ii) the slope of the phase boundary at the origin and (iii) the fact that the integrable impurity model at $J_1 = 1$, $J_2 = 0$ lies on the open$^-$–open$^+$ phase boundary.

We now discuss our numerical results on chains of length $L \leqslant 20$. We emphasize at the outset that we are fighting finite-size corrections that vanish logarithmically slowly from two sources: the bulk marginal coupling, g of section 3 which is present everywhere in the phase diagram and the marginal boundary operator λ which is present in some parts of the phase diagram. Thus we can only expect our results to be of qualitative value.

In figure 10 we present the scaled energy gaps, $L(E - E_{1^+})/2\pi v$, for the four states with quantum number $0^\pm$ and $1^\pm$ as a function of J_1 with J_2 fixed at $J_2 = 0$. In figure 10 the integrable impurity model thus corresponds to $J_1 = 1$.

First, let us consider what happens as we increase J_1 away from its value, $J_1 = 1$ at the integrable impurity model. We see that the 0^+–1^- gap drops rapidly with increasing J_1. This is to be expected since, according to figure 6 the system is in the open$^+$ phase. Note however, that the 0^+ state is not the ground-state, even for $J_1 \approx 4$, for $L \leqslant 20$. We do expect that it would become the ground-state for sufficiently large L, for any $J_1 > 1$. In figure 10 we show results for two different chain lengths $L = 8$ and $L = 20$. As can be seen there is some evidence that the 1^-–0^+ gap indeed is closing with increasing L. The scaled gaps between the $0^\pm - 1^\pm$ states become asymptotically degenerate at $J_1 = 1$, the integrable impurity model. As seen in figure 10 the 0^+ level has the most negative slope as a function of J_1. It is then plausible that as the gap closes at $J_1 = 1$, the 0^+ state crosses the 1^- state for $J_1 > 1$. Even for large J_1 this level-crossing only takes place at large L. The reason is that as $J_1 \to \infty$ for fixed L, we obtain the ground state of the three-spin cluster,

1^+, times the ground state for the rest of the (open) chain with two sites removed resulting in the 1^- ground state. Eventually, if J_1 is kept fixed, the effective $S = 1$ impurity is screened for long enough chains, producing the 0^+ ground state, but this process proceeds logarithmically slowly. Finite-size scaling analysis, although not very reliable due to the marginal operators, seems to indicate that J_2 is relevant, as expected.

Now consider what happens as we decrease J_1. At $J_1 = 0$ we obtain, approximately the open$^+$ $\times$ $(S = 1)$ spectrum, shown in table 1, as expected. Note also, the minimum in the 1^+–0^- gap which occurs for $J_1 \approx 0.7$. With increasing L we expect a crossing of these two levels to occur. Asymptotically the 0^- state should lie below the 1^+ state for all J_1 such that $0 < J_1 < 1$, since this region should be in the open$^-$ phase.

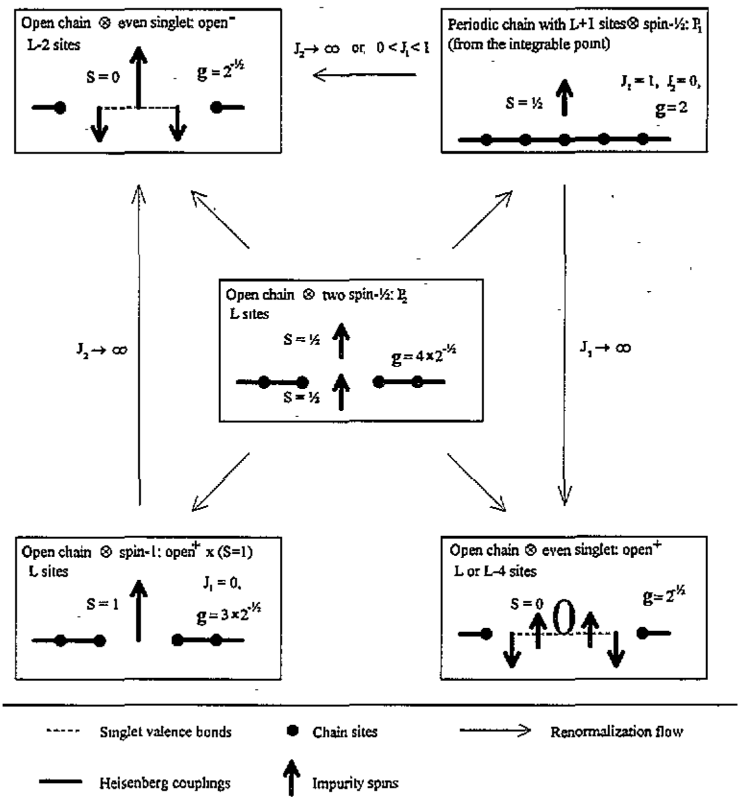

Figure 11. The five fixed points and the RG flows occurring in figure 6. '0' denotes the $S^z = 0$ state of the $S = 1$ impurity.

We now consider the effect of varying J_2 away from 0 with J_1 held fixed at its integrable value, $J_1 = 1$ (see figure 8). The open$^-$ spectrum of table 1 is obtained for large positive J_2, as expected. Although we expect to be in the open$^+$ $\times$ $(S = 1)$ phase for sufficiently large $J_2 < 0$, this is not obvious from figure 8. The problem is that, for $J_2 \to -\infty$ for fixed L the three-spin complex has an $S = 2$ ground state giving a 2^- ground state including the decoupled open chain. The screening of this $S = 2$ effective impurity down to $S = 1$ is logarithmically slow. Indeed, the open$^+$ $\times$ $(S = 1)$ spectrum is best approximated in this region for $J_2 \approx -0.3$. This may correspond to crossing the open$^-$–open$^+$ $\times$ $(S = 1)$ phase boundary, in figure 6 where the marginal boundary coupling vanishes.

According to the 'g-theorem' the 'ground-state degeneracy', g, decreases under renormalization from less stable to more stable fixed points [2]. The value of g for a periodic chain [6] is 1 and for an open chain is $1/\sqrt{2}$. These values must be multiplied by the degeneracy of the decoupled impurity at each critical point. Thus, at P_2, $g = 4/\sqrt{2}$; at P_1, $g = 2$, at the origin, $g = 3/\sqrt{2}$ and at the open$^+$ and open$^-$ critical points at ∞, $g = 1/\sqrt{2}$. We see that, in all cases, the g-theorem is obeyed. A pictorial summary of the five fixed points and the corresponding values of g are given in figure 11.

5. Conclusions

The apparent contradiction between the integrable model and our RG analysis is explained by the fact that this model renormalizes to an *unstable* critical point corresponding to a periodic chain with a decoupled $S = 1/2$ impurity. Our numerical analysis of the integrable impurity model, for $L \leqslant 5000$, establishes rather convincingly that it renormalizes, logarithmically slowly, to this unstable fixed point. Piecing together various bits of information using the renormalization group, we have hypothesized a general phase diagram. As discussed in the previous section, certain aspects of this phase diagram have been quite well established independently of the numerical work reported in that section. Others, such as the detailed shape of the open$^+$–open$^-$ and open$^+$–open$^+$ $\times$ ($S = 1$) phase boundaries at small values of the J_i's have not. These details must be investigated numerically. This numerical investigation is made difficult by the logarithmically slow finite-size convergence. Nevertheless, all the results obtained are consistent with our phase diagram; indeed using them we were able to make an approximate determination of a point on a phase boundary. Importantly, we were able to understand in detail why certain features of the thermodynamic limit are already evident for $L = 20$ and others are not.

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