# Analytical calculation of the finite-size crossover spectrum of the anisotropic two-channel Kondo model

Gergely Zaránd

Institute of Physics, Technical University of Budapest, H-1521 Budafoki út 8, Budapest, Hungary and International School for Advanced Studies, I-34014 Trieste, Italy

Jan von Delft

Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany (Received 10 December 1998; revised manuscript received 23 September 1999)

We present a conceptually simple, analytical calculation of the finite-size crossover spectrum of the anisotropic two-channel Kondo (2CK) model at its Toulouse point. We use Emery and Kivelson's method, generalized in two ways. First, we construct all boson fields and Klein factors explicitly in terms of the model's original fermion operators and, secondly, we clarify explicitly how the Klein factors needed when refermionizing act on the original Fock space. This enables us to follow the evolution of the 2CK model's free-fermion states to its exact eigenstates for arbitrary magnetic fields and spin-flip coupling strengths. We thus obtain an *analytic* description of the crossover of the finite-size spectrum to the non-Fermi-liquid fixed point, where we recover the conformal field theory results (implying a direct proof of Affleck and Ludwig's fusion hypothesis). From the finite-size spectrum we extract the operator content of the 2CK fixed point and the dimension of various relevant and irrelevant perturbations. Our method can easily be generalized to include various symmetry-breaking perturbations, and to study the crossover to other fixed points produced by these. Furthermore, it establishes instructive connections between different renormalization group schemes. We also apply our method to the single-channel Kondo model.

#### I. INTRODUCTION

One of the most intriguing aspects of a non-Fermi liquid (NFL) is that its elementary excitations are not simply related to the bare excitations of the non-interacting Fermi liquid; gaining an understanding of the nature of the elementary excitations of a NFL is thus an important conceptual challenge. The two-channel Kondo (2CK) model, introduced in 1980 by Nozières and Blandin,<sup>1</sup> is one of the simplest and most-studied quantum impurity models with NFL behavior, and offers the rare opportunity to address this question directly: it has both a free and a NFL fixed point, and the crossover between the two, including the change in the nature of the elementary excitations, can be analyzed exactly using the bosonization approach of Emery and Kivelson<sup>2</sup> (EK).

In the 2CK model two channels of spinful conduction electrons interact with a single spin 1/2 impurity via a local antiferromagnetic exchange interaction. In contrast to the single-channel Kondo (1CK) model, which has a stable infinite-coupling fixed point at which the conduction electrons screen the impurity spin completely, in the two-channel case the impurity spin is *overscreened* at infinite coupling, and the 2CK model's infinite-coupling fixed point is unstable. A stable NFL fixed point exists at intermediate coupling, and is characterized by a nonzero residual entropy and nonanalytical behavior for various physical quantities. The relevance of this model to physical systems is extensively reviewed in Ref. 3.

In this paper, we use EK's method to perform a conceptually simple, analytic calculation of the finite-size crossover spectrum of the 2CK model between the free and the NFL fixed points, a result first reported in Ref. 4. The calculation enables us to elucidate the nature of the NFL excitations at the fixed point in great and instructive detail, and to see explicitly how the symmetries of the NFL fixed point emerge as it is approached from the crossover region. Furthermore it establishes instructive connections between various popular renormalization group (RG) schemes, since it allows one to *analytically* illustrate their main ideas.

The two-channel Kondo model has of course already been studied theoretically by an impressive number of different methods, which are comprehensively reviewed in Ref. 3. They include approximate methods such as multiplicative<sup>1,5,6</sup> and path-integral<sup>7,8</sup> RG approaches and slave-boson methods;<sup>9–11</sup> effective models such as the so-called compactified model,<sup>12–15</sup> which is partially equivalent to the 2CK model; the numerical RG (NRG);<sup>16–18</sup> and exact methods, such as the Bethe ansatz,<sup>19–21</sup> conformal field theory (CFT),<sup>18,22–24</sup> and Abelian bosonization.<sup>2,4,25–30</sup>

Among the several exact approaches to solving the 2CK model, the one that in our opinion is the most simple and straightforward, is that introduced by Emery and Kivelson (EK),<sup>2</sup> who employ one-dimensional Abelian bosonization (pedagogically reviewed in Ref. 31) and refermionization to show that along the so-called Emery-Kivelson line (Toulouse point) the anisotropic 2CK model maps onto a *quadratic* resonant-level model. Since spin anisotropy is irrelevant for the 2CK Kondo model<sup>18</sup> (as also shown below), their work also yielded new insight into the generic behavior of the isotropic 2CK model.

Though the approach is constrained to the vicinity of the EK line, the latter is stable<sup>32</sup> and connects the Fermi-liquid and non-Fermi-liquid regimes, so that EK's method captures

PRB <u>61</u>

6918

©2000 The American Physical Society

both the model's NFL behavior and the crossover from the free to the NFL fixed point. EK calculated a number of thermodynamic and impurity properties and also some electron correlation functions, and explained the NFL behavior by the observation that only "one half" of the impurity's Majorana degrees of freedom couples to the electrons. Although at the EK line the properties of the model are somewhat specific since the leading irrelevant operator vanishes along it, the generic behavior can easily be derived by perturbation theory in its vicinity. The EK method has since been fruitfully applied and generalized to several related quantum impurity problems.<sup>25–29</sup> Ye in particular showed how to use the EK method and simple scaling arguments<sup>27</sup> to identify easily the fixed points of various bosonizable quantum impurity models, including the k-channel spin anisotropic Kondo model,<sup>27(a)</sup> and how to calculate electronic correlation functions at these fixed points.

In a recent publication,<sup>4</sup> we have shown that the power of EK-bosonization can actually be increased even more [see points (i)–(vi) and (x)–(xii) below] by generalizing it to *finite system size L*. Though retaining terms of order 1/L naturally requires some additional technical effort, none of the conceptual simplicity of the EK approach is thereby lost. The present paper is devoted to presenting the calculations by which the results of Ref. 4 were obtained in explicit detail, and includes discussions of a number of subtleties and results not mentioned there.

The generalization to finite system size necessitates two important modifications relative to the work of EK. (1) While they use the field-theoretical approach to bosonization in which the bosonization relation  $\psi_{\alpha j} \simeq F_{\alpha j} e^{-i\phi_{\alpha j}}$  is used merely as a formal correspondence, we use the more careful constructive bosonization procedure of Haldane,33,31 where both the boson fields  $\phi_{\alpha j}$  and Klein factors  $F_{\alpha j}$  are constructed *explicitly* from the original  $\psi_{\alpha i}$  operators, so that the bosonization formula becomes an operator identity in Fock space. (2) Since EK were interested mainly in impurity properties, they did not need to discuss at all the Klein factors  $F_{\alpha i}$  [which lower the number of  $\alpha j$  electrons by one and ensure proper anticommutation relations for the  $\psi_{\alpha i}$ 's]. However, as has been pointed out by several authors recently,<sup>28,31,34,35</sup> these Klein may be extremely important in some situations, and they are essential for quantities like the finite-size spectrum or various electron correlation functions.<sup>33,4</sup> Therefore it is crucial to specify how the new Klein factors of the refermionized operators act on the Fock space. As we shall see, these new Klein factors are only well defined on a suitably *enlarged* Fock space that also contains unphysical states, which must be discarded at the end using certain gluing conditions.

With these modifications, EK's bosonization approach enables us by straightforward diagonalization of the quadratic resonant-level model (i) to analytically calculate the crossover of the 2CK model's finite-size spectrum from the FL to the NFL fixed point, at which we reproduce the fixed-point spectrum previously found by CFT using a certain fusion hypothesis (which we thereby prove directly); (ii) to construct the eigenstates of the 2CK model corresponding to this crossover spectrum explicitly, thereby elucidating the nature of the NFL excitations; and (iii) to extract the operator content of the NFL fixed point and determine the dimensions of different relevant and irrelevant operators. We also prove that the leading irrelevant operator is missing along the EK line but is present away from it. Since our method works also in the presence of an arbitrary magnetic field (unlike CFT), we can also (iv) investigate how a finite magnetic field destroys the NFL spectrum for the low-energy excitations of the model and restores the FL properties. (v) Furthermore, our finite-size bosonization approach can easily be related to various popular RG methods; it therefore not only provides a useful bridge between them, but can potentially be used as a pedagogical tool for *analytically* illustrating their main ideas. (vi) For completeness, we also construct the analytical finite size spectrum of the *single channel Kondo model*, and calculate the crossover between its weak and strong coupling Fermi liquid fixed points.

In a future publication<sup>36</sup> we shall show that EK's method furthermore allows one (vii) to construct very easily the scattering states of the model; (viii) to verify explicitly the validity of the bosonic description of the NFL fixed point worked out in Refs. 30 and 27; (ix) to determine the fixed point boundary conditions at the impurity site for the different currents and fields in a very straightforward way, (x) as well as the leading corrections to these; (xi) to calculate all correlation functions at and around the NFL fixed point; and (xii) to clarify the role of the dynamics of Klein factors in correlation functions. [Although (vii) to (ix) can also be obtained in a system of infinite size, (x) to (xii) turn out to depend crucially on the finite-size results of the present paper.] This implies that all CFT results can be checked from first principles using bosonization.

The paper is organized as follows. In Sec. II we define the 2CK model to be studied. For completeness, and since the proper use of Klein factors is essential, Sec. III briefly reviews the "constructive" (operator identity-based) approach to finite-size bosonization used throughout this paper. The Emery-Kivelson mapping onto a resonant-level model is discussed in Sec. IV, using our novel, more explicit formulation of refermionization within a suitably extended Fock space. The solution of the resonant level model and the construction of the NFL spectrum using generalized gluing conditions is presented in Sec. V. In Sec. VI the results of our finite-size calculations are compared with and interpreted in terms of various RG procedures. In Sec. VII we show the finite-size spectrum for the 1CK model. Finally, in Sec. VIII we summarize our conclusions.

The centerpiece of the main text is our uncommonly careful and detailed finite-size formulation of the EK mapping. Technicalities not related to this mapping are relegated to four Appendixes (see Ref. 37). Appendix A discusses in some detail matters related to the choice of an ultraviolet cutoff, and also gives the often-used position-space definition of the 2CK model, to facilitate comparison with our momentum-space version. The construction of the extended Fock space needed for refermionization is discussed in Appendix B, and the technical details used to diagonalize the resonant-level model and to calculate several of its properties are given in Appendix C. Finally, in Appendix D we present our finite-size bosonization calculation for the one-channel Kondo model as well.

## **II. DEFINITION OF THE MODEL**

Throughout the main part of this paper we shall use the standard 2CK Hamiltonian in momentum space. We consider a magnetic impurity with spin 1/2 placed at the origin of a sphere of radius R = L/2, filled with two species of free, spinful conduction electrons, labeled by a spin index  $\alpha = (\uparrow, \downarrow) = (+, -)$  and a channel or flavor index j = (1,2) = (+, -). We assume that the interaction between the impurity and the conduction electron is sufficiently short-ranged that it involves only *s*-wave conduction electrons, whose kinetic energy can be written as

$$H_0 = \sum_{k\alpha j} k: c^{\dagger}_{k\alpha j} c_{k\alpha j}: \quad (v_F = \hbar = 1).$$
 (1)

The operator  $c_{k\alpha j}^{\dagger}$  creates an *s*-wave conduction electron of species  $(\alpha j)$  with radial momentum  $k \equiv p - p_F$  relative to the Fermi momentum  $p_F$ , and the dispersion has been linearized around the Fermi energy  $\varepsilon_F : \varepsilon_k - \varepsilon_F \approx k$ . The colons in Eq. (1) denote normal ordering with respect to the free Fermi sea or "vacuum state"  $|\vec{0}\rangle_0$ :

$$c_{k\alpha i}|0\rangle_0 \equiv 0 \quad \text{for} \quad k > 0,$$
 (2a)

$$c_{k\alpha i}^{\dagger} | \vec{0} \rangle_0 \equiv 0 \quad \text{for} \quad k \leq 0.$$
 (2b)

The  $c_{k\alpha j}$ 's obey standard anticommutation relations  $\{c_{k\alpha j}, c^{\dagger}_{k'\alpha' j'}\} = \delta_{kk'} \delta_{\alpha \alpha'} \delta_{jj'}$ , where due to radial momentum quantization the values of *k* are quantized:

$$k = \frac{2\pi}{L} (n_k - P_0/2), \quad n_k \in \mathbb{Z}.$$
 (3)

Here  $P_0=0$  or 1, since at zero temperature the chemical potential (and hence  $p_F$ ) must either coincide with a degenerate level ( $P_0=0$ ) or lie midway between two of them ( $P_0=1$ ). The level spacing in both cases is

$$\Delta_L = 2 \pi / L. \tag{4}$$

The *s*-wave conduction electrons can also be described by a one-dimensional chiral field  $^{23(b)}$ 

$$\psi_{\alpha j}(x) \equiv \sqrt{\frac{2\pi}{L}} \sum_{n_k \in \mathbb{Z}} e^{-ikx} c_{k\alpha j}, \qquad \left( x \in \left[ -\frac{L}{2}, \frac{L}{2} \right] \right),$$
(5)

$$\{\psi_{\alpha j}(x), \psi^{\dagger}_{\alpha' j'}(x')\} = \delta_{\alpha \alpha'} \delta_{jj'} 2 \pi \delta(x - x').$$
(6)

In the continuum limit  $L \rightarrow \infty$ , the x > 0 and x < 0 portions of  $\psi_{\alpha j}(x)$  can be associated with the incoming and outgoing scattering states, respectively. Note that for  $P_0=0$  or 1 the fields  $\psi_{\alpha j}(x)$  have periodic or antiperiodic boundary conditions at  $x = \pm L/2$ , respectively, hence  $P_0$  will be called the "periodicity parameter."

We assume a short-ranged anisotropic exchange interaction between the impurity spin and the *s*-wave conduction electron spin density at the origin of the form

$$H_{\text{int}} = \Delta_L \sum_{\substack{\mu,k,k'\\\alpha,\alpha',j}} \lambda_{\mu} S_{\mu} : c_{k\alpha j}^{\dagger} \left( \frac{1}{2} \sigma_{\alpha \alpha'}^{\mu} \right) c_{k' \alpha' j} : .$$
(7)

Here the  $S_{\mu}$  ( $\mu = x, y, z$ ) are the impurity spin operators, with  $S_z$  eigenvalues  $(\uparrow, \downarrow) = (\frac{1}{2}, -\frac{1}{2})$ , and the  $\lambda_{\mu}$ 's denote dimensionless couplings:  $\lambda_z$  generates different phase shifts for spin-up and spin-down conduction electrons, while  $\lambda_x \equiv \lambda_y \equiv \lambda_{\perp}$  describe spin-flip scattering off the impurity. Finally, we add a magnetic term

$$H_h = h_i S_z + h_e \hat{\mathcal{N}}_s, \qquad (8)$$

where  $h_i$  and  $h_e$  denote the magnetic fields acting on the impurity and conduction electron spins, respectively, and  $\hat{\mathcal{N}}_s$  denotes the total spin of the conduction electrons.

Since the constructive bosonization method requires an unbounded spectrum, the fermion bandwidth cutoff is removed (i.e., taken to be infinite) in the equations above. This ultraviolet cutoff will only be restored when we define the new Bose fields in Eq. (13) below.

## **III. BOSONIZATION BASICS**

The key to diagonalizing the Hamiltonian is to find the relevant quantum numbers of the problem and to bosonize the Hamiltonian carefully. While bosonization is a widely used technique, the so-called Klein factors mentioned in the Introduction are often neglected or not treated with sufficient care. In the present section we therefore discuss our bosonization approach in somewhat more detail than usual, formulating it as a set of *operator identities in Fock space*, and emphasizing in particular the proper use of Klein factors to ladder between states with different particle numbers in Fock space.

#### A. Bosonization ingredients

As a first step we introduce the operators

$$\hat{N}_{\alpha j} \equiv \sum_{k} : c^{\dagger}_{k\alpha j} c_{k\alpha j} :, \qquad (9)$$

which count the number of electrons in channel  $(\alpha j)$  with respect to the free electron reference ground state  $|\vec{0}\rangle_0$ . The nonunique eigenstates of  $\hat{N}_{\alpha j}$  will generically be denoted by  $|\vec{N}\rangle \equiv |N_{\uparrow 1}\rangle \otimes |N_{\downarrow 1}\rangle \otimes |N_{\uparrow 2}\rangle \otimes |N_{\downarrow 2}\rangle$ , where the  $N_{\alpha j}$ 's can be arbitrary integers, i.e.,  $\vec{N} \in \mathbb{Z}^4$ .

Next, we define bosonic electron-hole creators by

$$b_{q\alpha j}^{\dagger} \equiv \frac{i}{\sqrt{n_q}} \sum_{n_k \in \mathbb{Z}} c_{k+q\alpha j}^{\dagger} c_{k\alpha j}, \qquad (10)$$

where  $q = 2\pi n_q/L > 0$  and the  $n_q$  are positive integers. The operators  $b_{q\alpha j}^{\dagger}$  create "density excitations" with momentum q in channel  $\alpha j$ , satisfy standard bosonic commutation relations, and commute with the  $\hat{N}_{\alpha i}$ 's:

$$\begin{bmatrix} b_{q\alpha j}, b_{q'\alpha' j'}^{\dagger} \end{bmatrix} = \delta_{qq'} \delta_{\alpha \alpha'} \delta_{jj'}, \quad \begin{bmatrix} b_{q\alpha j}, \hat{N}_{\alpha' j'} \end{bmatrix} = 0.$$
(11)

Among all states  $|\vec{N}\rangle$  with given  $\vec{N}$ , there is a unique state, to be denoted by  $|\vec{N}\rangle_0$ , that contains *no holes* and thus has the defining property

PRB <u>61</u>

$$b_{q\alpha j}|N\rangle_0 = 0$$
 (for any  $q > 0, \alpha, j$ ). (12)

We shall call it the " $\tilde{N}$ -particle ground state," since in the absence of interactions no  $|\vec{N}\rangle$  has a lower energy than  $|\vec{N}\rangle_0$ ; likewise, no  $|\vec{N}\rangle_0$  has a lower energy than the "vacuum state"  $|\vec{0}\rangle_0$  defined in Eq. (2). Note, though, that if  $P_0=0$ , the states  $c_{0\alpha j}|\vec{0}\rangle_0$  are degenerate with  $|\vec{0}\rangle_0$ , because then  $c_{0\alpha j}$  removes a zero-energy electron. Any  $\vec{N}$ -electron state  $|\vec{N}\rangle$  can be written as  $|\vec{N}\rangle = f(b^{\dagger})|\vec{N}\rangle_0$ , i.e., by acting on the  $\vec{N}$ -electron ground state with an appropriate function of electron-hole creation operators.<sup>33,31</sup>

Next, we define bosonic fields by

$$\phi_{\alpha j}(x) \equiv \sum_{q>0} \frac{-1}{\sqrt{n_q}} (e^{-iqx} b_{q\alpha j} + e^{iqx} b_{q\alpha j}^{\dagger}) e^{-aq/2}.$$
 (13)

Here  $a \sim 1/p_F$  is a short-distance cutoff; it is introduced to cure any ultraviolet divergences the theory may have acquired by taking the fermion bandwidth to be infinite. It is well known, however, that within this *bosonization cutoff scheme* the coupling constants have different meanings than for other standard regularization schemes using a finite fermion bandwidth, and that the relations between coupling constants in different regularization schemes can be found by requiring that they yield the same phase shifts. This and other cutoff related matters are discussed in Appendix A.<sup>37</sup> The fields  $\partial_x \phi_{\alpha j}(x)$  are canonically conjugate to the  $\phi_{\alpha i}(x)$ 's

$$\begin{bmatrix} \phi_{\alpha j}(x), \partial_{x'} \phi_{\alpha' j'}(x') \end{bmatrix} = 2\pi i (\delta_a(x-x')-1/L) \delta_{\alpha \alpha'} \delta_{jj'},$$
(14)

where  $\delta_a(x) = a/\pi(x^2 + a^2)$  is the smeared delta function.

As final bosonization ingredient, we need the so-called Klein factors  $F_{\alpha j}$ , which ladder between states with different  $N_{\alpha j}$ 's. By definition, the  $F_{\alpha j}$ 's are required to satisfy the following relations:

[

$$[F_{\alpha j}, \hat{N}_{\alpha' j'}] = \delta_{\alpha \alpha'} \delta_{jj'} F_{\alpha j}, \qquad (15a)$$

$$F_{\alpha j}, b_{q \alpha' j'}] = [F_{\alpha j}, b_{q \alpha' j'}^{\dagger}] = 0, \qquad (15b)$$

$$F_{\alpha j}F_{\alpha j}^{\dagger} = F_{\alpha j}^{\dagger}F_{\alpha j} = 1, \qquad (15c)$$

$$\{F_{\alpha j}, F_{\alpha' j'}^{\dagger}\} = 2\,\delta_{\alpha \alpha'}\,\delta_{jj'} \tag{15d}$$

$$\{F_{\alpha j}, F_{\alpha' j'}\} = 0 \quad \text{for } (\alpha j) \neq (\alpha' j').$$
(15e)

These relations imply that  $F_{\alpha j}$  ( $F_{\alpha j}^{\dagger}$ ) decreases (increases) the electron number in channel { $\alpha j$ } by one without creating particle-hole excitations. As shown in Refs. 33 or 31, the construction  $F_{\alpha j} = a^{1/2} \psi_{\alpha j}(0) e^{i\phi_{\alpha j}(0)}$ , which explicitly expresses  $F_{\alpha j}$  in terms of the fermion operators  $c_{k\alpha j}$ , has all the desired properties.

#### **B.** Bosonization identities

Any expression involving the fermion operators  $c_{k\alpha j}$  can be rewritten in terms of the the Klein factors  $F_{\alpha j}$  and boson fields  $\phi_{\alpha j}$  defined above. In our notation, the standard bosonization identities<sup>33</sup> for the fermion field, density and kinetic energy take the following forms:<sup>31</sup>

$$\psi_{\alpha j}(x) = F_{\alpha j} a^{-1/2} e^{-i(\hat{N}_{\alpha j} - P_0/2)2\pi x/L} e^{-i\phi_{\alpha j}(x)}, \quad (16)$$

$$\frac{1}{2\pi}:\psi^{\dagger}_{\alpha j}(x)\psi_{\alpha j}(x):=\frac{1}{2\pi}\partial_x\phi_{\alpha j}(x)+\hat{N}_{\alpha j}/L,\qquad(17)$$

$$H_{0} = \sum_{\alpha j} \frac{\Delta_{L}}{2} \hat{N}_{\alpha j} (\hat{N}_{\alpha j} + 1 - P_{0}) + \sum_{\substack{\alpha j \\ q > 0}} q b_{q \alpha j}^{\dagger} b_{q \alpha j}.$$
(18)

Several comments are in order: (i) in the limit  $a \rightarrow 0$  Eqs. (16) to (18) are not mere formal correspondences between the fermionic and bosonic expressions, but hold as rigorous operator identities in Fock space. For  $a \neq 0$ , they should be viewed as conveniently regularized redefinitions of the fermion fields and densities (see<sup>37</sup> Appendix A 2). (ii) The Klein factors  $F_{\alpha j}$  in Eq. (16) play a twofold role: First, by Eq. (15a) they ensure that the right-hand side of Eq. (16) acting on any state indeed does lower the number of  $\alpha j$ electrons by one, just as  $\psi_{\alpha j}$  does; and secondly, by Eqs. (15d) and (15e) they ensure that fields with different  $(\alpha j)$ 's do have the proper anticommutation relations (6). (iii) In Eqs. (18) the first  $\Delta_L$  term is just  $\sqrt[6]{N}|H_0|\tilde{N}\rangle_0$ , the energy of the  $\vec{N}$ -particle ground state  $|\vec{N}\rangle_0$  relative to  $|\vec{0}\rangle_0$ . Since the Klein factors do not commute with this term, they evidently cannot be neglected when calculating the full model's finitesize spectrum, for which all terms of order  $\Delta_L$  must be retained. The second term of Eq. (18) describes the energy of electron-hole excitations relative to  $|\vec{0}\rangle_0$ .

#### **IV. EMERY-KIVELSON MAPPING**

In this section, we map the 2CK model onto a resonant level model, using a finite-size version of the strategy invented by Emery and Kivelson: using bosonization and refermionization, we make a unitary transformation to a more convenient basis, in which the Hamiltonian is quadratic for a certain choice of parameters.

#### A. Conserved quantum numbers

The quantum numbers  $N_{\alpha j}$  of Eq. (9) are conserved under the action of  $H_0$ ,  $H_h$ , and  $H_z$  (the  $\lambda_z$  term of  $H_{int} \equiv H_z$  $+H_{\perp}$ ), but fluctuate under the action of the spin-flip interaction  $H_{\perp}$  (the  $\lambda_{\perp}$  term). On the other hand, the total charge and flavor of the conduction electrons is obviously conserved by all terms in the Hamiltonian, including  $H_{\perp}$ . Therefore it is natural to introduce the following new quantum numbers:

where  $2\hat{\mathcal{N}}_c$ ,  $\hat{\mathcal{N}}_s$ , and  $\hat{\mathcal{N}}_f$  denote the total charge, spin, and flavor of the conduction electrons, and  $\hat{\mathcal{N}}_x$  measures the spin difference between channels 1 and 2. Clearly, any conduc-



FIG. 1. Under a succession of spin flips,  $N_s$  fluctuates *mildly* between  $S_T \neq 1/2$  (here  $S_T = 1/2$ ); in contrast,  $N_x$  fluctuates *wildly*, since it can acquire *any* value consistent with the gluing conditions (20). The dotted line represents the reference energy 0 up to which the free Fermi sea is filled for  $P_0 = 1$ , the filled and empty circles represent filled and empty single-particle states with energy k, which increases from left to right.

tion electron state  $|\tilde{N}\rangle$  can equally well be labeled by the corresponding quantum numbers  $\tilde{\mathcal{N}} \equiv (\mathcal{N}_c, \mathcal{N}_s, \mathcal{N}_f, \mathcal{N}_x)$ . However, whereas the  $N_{\alpha j}$ 's take arbitrary independent integer values, the  $\tilde{\mathcal{N}}$ 's generated by Eq. (19) (with  $\tilde{N} \in \mathbb{Z}^4$ ) can easily be shown to satisfy the following *free gluing conditions*:

$$\vec{\mathcal{N}} \in (\mathbb{Z} + P/2)^4, \tag{20a}$$

$$\mathcal{N}_c \pm \mathcal{N}_f = (\mathcal{N}_s \pm \mathcal{N}_x) \mod 2,$$
 (20b)

where the *parity index P* equals 0 or 1 if the total number of electrons is even or odd, respectively. Equation (20a) formalizes the fact that the addition or removal of one  $\alpha j$  electron to or from the system changes *each* of the  $\mathcal{N}_y$ 's by  $\pm 1/2$ , so that they are either all integers or all half-integers. Equation (20b) selects from the set of all  $\mathcal{N}$  of the form (20a) the physical ones for which  $\mathcal{N} \in \mathbb{Z}^4$ , and eliminates the unphysical ones for which  $\mathcal{N} \in (\mathbb{Z} + 1/2)^4$ .

In the new basis,  $N_c$  and  $N_f$  are conserved; moreover,  $N_s$ fluctuates only "mildly" between the values  $S_T \mp 1/2$ , since the total spin

$$S_T \equiv \mathcal{N}_s + S_z \tag{21}$$

is conserved. In contrast,  $\mathcal{N}_x$  fluctuates "wildly," because an appropriate succession of spin flips can produce any  $\mathcal{N}_x$  that satisfies Eq. (20b), as illustrated in Fig. 1. This wildly fluctuating quantum number will be seen below to be at the heart of the 2CK model's NFL behavior. In revealing contrast, the 1CK model, which shows no NFL behavior, lacks such a wildly fluctuating quantum number (see Appendix D).

Since  $S_T$ ,  $N_c$ , and  $N_f$  are conserved, the Fock space  $\mathcal{F}_{phys}$  of all physical states can evidently be divided as follows into subspaces invariant under the action of *H*:

$$\mathcal{F}_{\text{phys}} = \sum_{\oplus 'S_T, \mathcal{N}_c, \mathcal{N}_f} \mathcal{S}_{\text{phys}}(S_T, \mathcal{N}_c, \mathcal{N}_f), \qquad (22)$$

$$\mathcal{S}_{\text{phys}}(S_T, \mathcal{N}_c, \mathcal{N}_f) = \sum_{\oplus '\mathcal{N}_x} \{ |\mathcal{N}_c, S_T - 1/2, \mathcal{N}_f, \mathcal{N}_x; \uparrow \rangle \\ \oplus |\mathcal{N}_c, S_T + 1/2, \mathcal{N}_f, \mathcal{N}_x + 1; \downarrow \rangle \}.$$
(23)

In both equations the prime on the sum indicates a restriction to those  $\mathcal{N}_{y}$ 's that satisfy the free gluing conditions (20). To

diagonalize the Hamiltonian for given  $S_T$ ,  $\mathcal{N}_c$ , and  $\mathcal{N}_f$ , it evidently suffices to restrict one's attention to the corresponding subspace  $S_{\text{phys}}(S_T, \mathcal{N}_c, \mathcal{N}_f)$ .

## **B. Emery-Kivelson transformation**

Following Emery and Kivelson, we now introduce, in analogy to Eq. (19), new electron-hole operators and boson fields via the transformations

$$\left. \begin{array}{l} b_{qy} \equiv \sum_{\alpha j} R_{y,\alpha j} b_{q\alpha j} \\ \varphi_{y} \equiv \sum_{\alpha j} R_{y,\alpha j} \phi_{\alpha j} \end{array} \right\} \qquad (y = c, s, f, x), \qquad (24)$$

where  $R_{y,\alpha j}$  is the unitary matrix in Eq. (19). These obey relations analogous to Eqs. (11) and (14), with  $\alpha j \rightarrow y$ . Moreover, we define  $|\tilde{\mathcal{N}}\rangle_0$ , the  $\tilde{\mathcal{N}}$ -particle vacuum state, to satisfy  $b_{qy}|\tilde{\mathcal{N}}\rangle_0=0$ , as in Eq. (12). If  $\tilde{\mathcal{N}}$  and  $\tilde{\mathcal{N}}$  are related by Eq. (19), then the states  $|\tilde{\mathcal{N}}\rangle_0$  and  $|\tilde{\mathcal{N}}\rangle_0$  are equal up to an unimportant phase (see<sup>37</sup> Appendix B), because both have the same  $\hat{N}_{\alpha j}$  and  $\hat{\mathcal{N}}_y$  eigenvalues and both are annihilated by all  $b_{q\alpha j}$ 's and  $b_{qy}$ 's.

Using the quantum numbers  $\hat{\mathcal{N}}_y$  and the bosonic fields  $\varphi_y(x)$ , the  $H_0$  of Eq. (18) becomes

$$H_{0} = \Delta_{L} \left[ \hat{\mathcal{N}}_{c}(1 - P_{0}) + \sum_{y} \hat{\mathcal{N}}_{y}^{2} / 2 \right] + \sum_{y, q \geq 0} q b_{qy}^{\dagger} b_{qy},$$
(25)

while Eqs. (17) and (16) are used to obtain, respectively,

ł

$$H_{z} = \lambda_{z} [\partial_{x} \varphi_{s}(0) + \Delta_{L} \tilde{\mathcal{N}}_{s}] S_{z}, \qquad (26)$$
$$H_{\perp} = \frac{\lambda_{\perp}}{2a} [e^{-i\varphi_{s}(0)} S_{+} (F_{\perp 1}^{\dagger} F_{\uparrow 1} e^{-i\varphi_{x}(0)} + F_{\perp 2}^{\dagger} F_{\uparrow 2} e^{i\varphi_{x}(0)}) + \text{H.c.}]. \qquad (27)$$

Equations (25)–(27) and (8) constitute the bosonized form of the Hamiltonian for the anisotropic 2CK model, *up to and including terms of order*  $\Delta_L$ .

Next we simplify  $H_z$ . It merely causes a phase shift in the spin sector, which can be obtained explicitly using a unitary transformation (due to EK) parametrized by a real number  $\gamma$ , to be determined below:

$$H \rightarrow H' = UHU^{\dagger}, \quad U \equiv e^{i\gamma S_z \varphi_s(0)}.$$
 (28)

The impurity spin, spin-diagonal part of H, spin boson field and fermion fields then transform as follows (using, e.g., the identities in Appendix C of Ref. 31):

$$S_{\pm} \rightarrow U S_{\pm} U^{\dagger} = e^{\pm i \gamma \varphi_{s}(0)} S_{\pm} , \qquad (29)$$

$$H_0 + H_z \rightarrow H_0 + (\lambda_z - \gamma) \partial_x \varphi_s(0) S_z + \lambda_z \Delta_L \hat{\mathcal{N}}_s S_z + \gamma^2 [1/(4a) - \pi/(4L)], \qquad (30)$$

$$\varphi_s(x) \rightarrow \varphi_s(x) - 2\gamma S_z \arctan(x/a) \quad (|x| \leq L), \quad (31)$$

$$\psi_{\alpha i}(x) \to \psi_{\alpha i}(x) e^{i \alpha \gamma S_z \arctan(x/a)} \quad (|x| \ll L).$$
(32)

PRB <u>61</u>

Equation (30) is most easily derived in the momentum-space representation, but for Eq. (31), the position-space representation is more convenient [first evaluate  $U\partial_x\varphi_s(x)U^{-1}$  using Eq. (14), then integrate]. Equation (32) follows from Eq. (31), since  $\psi_{\alpha j} \propto e^{-i\alpha\varphi_s/2}$ .

Recalling that  $\partial_x \varphi_s(x)/2\pi$  contributes to the conduction electron spin density, we note by differentiating Eq. (31) that the EK transformation produces a change in the spin density of  $-2\gamma S_z \pi \delta_a(x)/2\pi$ , and thus ties a spin of  $-\gamma S_z$  from the conduction band to the impurity spin  $S_z$ .

To eliminate the  $S_z \partial_x \varphi_s$  term in Eq. (30), we now choose  $\gamma \equiv \lambda_z$ ; then the spin-flip-independent part of the Hamiltonian takes the form

$$H'(\lambda_{\perp}=0) = \lambda_z \Delta_L \hat{\mathcal{N}}_s S_z + \sum_y \Delta_L \hat{\mathcal{N}}_y^2 / 2 + \sum_{y, q \ge 0} q b_{qy}^{\dagger} b_{qy}$$
  
+  $H_h + \text{const},$  (33)

and  $H'_{\perp}$  contains the factors  $e^{\pm i(1-\lambda_z)\varphi_s(0)}$ . These factors are simply equal to 1 at the *Emery-Kivelson line*  $\lambda_z = 1$ , where  $H'_{\perp}$  simplifies to

$$H'_{\perp} = \frac{\lambda_{\perp}}{2a} \left[ S_{+} (F^{\dagger}_{\downarrow 1} F_{\uparrow 1} e^{-i\varphi_{\chi}(0)} + F^{\dagger}_{\downarrow 2} F_{\uparrow 2} e^{i\varphi_{\chi}(0)}) + \text{H.c.} \right].$$
(34)

We shall henceforth focus on the case  $\lambda_z = 1$ , which will enable us to diagonalize the model exactly by refermionization. Deviations from the EK line will be shown in Sec. VI C to be irrelevant, by taking  $\gamma = 1$  but  $\lambda_z = 1 + \delta \lambda_z$ , and doing perturbation theory in

$$\delta H'_{z} = \delta \lambda_{z} [\partial_{x} \varphi_{s}(0) + \Delta_{L} \hat{\mathcal{N}}_{s}] S_{z}.$$
(35)

The crucial property of the EK line is that it contains the NFL intermediate-coupling fixed point. A Heuristic way to see this it to note that on the EK line, the impurity spin is in fact "perfectly screened:" the spin  $-\gamma S_z$  from the conduction band, that is tied to the impurity by the EK transformation, is equal to  $-S_z$  if  $\gamma = \lambda_z = 1$ . It thus precisely "cancels" the impurity's spin  $S_z$ , and forms a "perfectly screened singlet" with zero total spin (without breaking channel symmetry), in agreement with the heuristic arguments of Nozières and Blandin.<sup>1</sup>

Of course, there are more rigorous ways of seeing that the NFL fixed point lies on the EK line. First, for  $\lambda_z = 1$  it follows from Eq. (32) that the phase shift  $\delta$  of the outgoing relative to the incoming fields, defined by  $\psi_{\alpha j}(0^-) \equiv e^{i2\delta}\psi_{\alpha j}(0^+)$  (with  $|0^{\pm}| \ge a$ ), is  $|\delta| = \pi/4$ , which is just the value known for the NFL fixed point from other approaches.<sup>7,18</sup> Secondly, we shall deduce in Sec. VI C from an analysis of the finite-size spectrum that the leading irrelevant operators with dimensions 1/2 vanish exclusively *along* this line, but not away from it. Since the presence or absence of the leading irrelevant operators strongly influences the low-temperature properties of the model such as its critical exponents,<sup>2,26</sup> and since these must stay invariant under any RG transformation, one concludes that the Emery-Kivelson line must be stable under RG transformations.

#### C. Refermionization

## 1. Definition of new Klein factors

The most nontrivial step in the solution of the model is the proper treatment of Klein factors when refermionizing the transformed Hamiltonian. In their original treatment EK did not discuss Klein factors at all and simply identified  $e^{-i\varphi_x(x)}/\sqrt{a}$  as a new pseudofermion field  $\psi_x(x)$ . Though this was adequate for their purposes, the proper consideration of the Klein factors and gluing conditions is essential for solving the model rigorously and obtaining the finite-size spectrum. Other authors tried to improve the Emery-Kivelson procedure by representing the Klein factors by  $F_{\alpha j} \sim e^{-i\Theta_{\alpha j}}$ , where  $\Theta_{\alpha j}$  is a "phase operator conjugate to  $\hat{N}_{\alpha j}$ ," and added these to the bosonic fields  $\phi_{\alpha j}$  before making the linear transformation (24). This procedure is problematic, however, since then  $e^{-i\varphi_y(0)}$  contains factors such as  $e^{-i\Theta_{\alpha j}/2}$ , which are ill defined (see Appendix D 2 of Ref. 31).

A rigorous way of dealing with Klein factors when refermionizing was presented in Ref. 4 (and adapted in Ref. 31 to treat an impurity in a Luttinger liquid): We introduce a set of ladder operators  $\mathcal{F}_y^{\dagger}$  and  $\mathcal{F}_y$  (y=c,s,f,x) to raise or lower the quantum numbers  $\mathcal{N}_y$  by  $\pm 1$ , with, by definition, the following properties:

$$[\mathcal{F}_{y}, \hat{\mathcal{N}}_{y'}] = \delta_{yy'} \mathcal{F}_{y}, \qquad (36a)$$

$$[\mathcal{F}_{y}, b_{qy'}] = [\mathcal{F}_{y}, b_{qy'}^{\dagger}] = 0, \qquad (36b)$$

$$\mathcal{F}_{y}\mathcal{F}_{y}^{\dagger} = \mathcal{F}_{y}^{\dagger}\mathcal{F}_{y} = 1, \qquad (36c)$$

$$\{\mathcal{F}_{y}, \mathcal{F}_{y'}^{\dagger}\} = 2 \,\,\delta_{yy'}, \qquad (36d)$$

$$\{\mathcal{F}_{y},\mathcal{F}_{y'}\}=0 \quad \text{for } y\neq y'.$$
(36e)

Now, note that the action of any one of the new Klein factors  $\mathcal{F}_y$  or  $\mathcal{F}_y^{\dagger}$  respects the first of the free gluing conditions (20a), but not the second, Eq. (20b). More generally, Eq. (20b) is respected only by products of an *even* number of new Klein factors, but violated by products of an *odd* number of them. This implies that the physical Fock space  $\mathcal{F}_{phys}$  of all  $|\tilde{\mathcal{N}}\rangle$  satisfying both Eqs. (20a) and (20b) is closed under the action of even but not of odd products of new Klein factors. *The action of arbitrary combinations of new Klein factors thus generates an extended Fock space*  $\mathcal{F}_{ext}$ , which contains  $\mathcal{F}_{phys}$  as a subspace and is spanned by the set of *all*  $|\tilde{\mathcal{N}}\rangle$  satisfying Eq. (20a), including unphysical states violating Eq. (20b). In Appendix B we show that  $\mathcal{F}_{phys}$  can indeed be embedded in  $\mathcal{F}_{ext}$ .<sup>37</sup>

Since odd products of  $\mathcal{F}_y$ 's lead out of  $\mathcal{F}_{phys}$ , they cannot be expressed in terms of the original Klein factors  $F_{\alpha j}$ , which leave  $\mathcal{F}_{phys}$  invariant. However, the Hamiltonian contains only even products of old Klein factors. Now, any combination  $F^{\dagger}_{\alpha j}F_{\alpha' j'}$  or  $F^{\dagger}_{\alpha j}F^{\dagger}_{\alpha' j'}$  of Klein factors just changes two of the  $N_{\alpha j}$  quantum numbers. Using Eq. (19) to read off the corresponding changes in  $\mathcal{N}_y$ , we can thus make the following identifications between pairs of the old and new Klein factors:

$$\mathcal{F}_{x}^{\dagger}\mathcal{F}_{s}^{\dagger} \equiv F_{\uparrow 1}^{\dagger}F_{\downarrow 1}, \quad \mathcal{F}_{x}\mathcal{F}_{s}^{\dagger} \equiv F_{\uparrow 2}^{\dagger}F_{\downarrow 2}, \qquad (37a)$$

$$\mathcal{F}_{x}^{\dagger}\mathcal{F}_{f}^{\dagger} \equiv F_{\uparrow 1}^{\dagger}F_{\uparrow 2}, \quad \mathcal{F}_{c}^{\dagger}\mathcal{F}_{s}^{\dagger} = F_{\uparrow 1}^{\dagger}F_{\uparrow 2}^{\dagger}.$$
(37b)

These relations, which each involve an arbitrary choice of sign, can be used to express any product of two old Klein factors in terms of two new ones, e.g.,  $\mathcal{F}_s^{\dagger} \mathcal{F}_f^{\dagger} = -(\mathcal{F}_x \mathcal{F}_s^{\dagger})(\mathcal{F}_x^{\dagger} \mathcal{F}_f^{\dagger}) = F_{\uparrow 1}^{\dagger} F_{\downarrow 2}$ . Since relations (37) by construction respect Eq. (19) (as can be checked by acting on any  $|\vec{N}\rangle$ ), they, and all similar bilinear relations derived from them, also respect both free gluing conditions (20).

We can thus replace the Klein factor pairs occurring in Eq. (34) by the ones in Eq. (37a):

$$H'_{\perp} = \frac{\lambda_{\perp}}{2a} [S_{+}F_{s}(F_{x}e^{-i\varphi_{x}(0)} + F_{x}^{\dagger}e^{i\varphi_{x}(0)}) + \text{H.c.}]. \quad (38)$$

The only consequence of this change is that we now work in the extended Fock space  $\mathcal{F}_{ext}$ , and will diagonalize H' not in the physical invariant subspace  $\mathcal{S}_{phys}(S_T, \mathcal{N}_c, \mathcal{N}_f)$  of Eq. (23), but in the corresponding extended subspace  $\mathcal{S}_{ext}(S_T, \mathcal{N}_c, \mathcal{N}_f)$ , given by an equation similar to Eq. (23), but with the  $\oplus' \mathcal{N}_x$  sum now restricted only to satisfy Eq. (20a), not also Eq. (20b). At the end of the calculation we shall then use the gluing condition (20b) to discard unphysical states. This approach is completely analogous to the use of gluing conditions in AL's CFT solution of the 2CK model. It is also somewhat analogous to Abrikosov's pseudofermion technique<sup>38</sup> of representing a spin operator via pseudofermions acting in an enlarged Hilbert space, and projecting out unphysical states at the end.

## 2. Pseudofermions and refermionized Hamiltonian

We now note that  $H'_{\perp}$  of Eq. (38) can be written in a form *quadratic* in fermionic variables

$$H'_{\perp} = \frac{\lambda_{\perp}}{2\sqrt{a}} [\psi_x(0) + \psi_x^{\dagger}(0)] (c_d - c_d^{\dagger}), \qquad (39)$$

by defining a local pseudofermion  $c_d$  and a pseudofermion field  $\psi_x(x)$  by the following refermionization relations:

$$c_d \equiv F_s^{\dagger} S_-, \quad c_d^{\dagger} c_d = S_z + 1/2,$$
 (40)

$$\psi_x(x) \equiv F_x a^{-1/2} e^{-i(\hat{\mathcal{N}}_x - 1/2)2 \pi x/L} e^{-i\varphi_x(x)}$$
(41a)

$$\equiv \sqrt{\frac{2\pi}{L}} \sum_{\bar{k}} e^{-i\bar{k}x} c_{\bar{k}x}, \qquad (41b)$$

where Eq. (41b) defines the  $c_{\bar{k}x}$  as Fourier coefficients of the field  $\psi_x(x)$ . For reasons discussed below, the field  $\psi_x$  in Eq. (41a) has been defined in such a way that its boundary condition at  $\pm L/2$  is *P* dependent, since  $\mathcal{N}_x \in \mathbb{Z} + P/2$  and  $\varphi_x(x)$  is a periodic function. Thus the quantized  $\bar{k}$  momenta in the Fourier expansion (41b) must have the form

$$\overline{k} = \Delta_L[n_{\overline{k}} - (1 - P)/2] \quad (n_{\overline{k}} \in \mathbb{Z}).$$

$$\tag{42}$$

The new pseudofermions were constructed in such a way that they satisfy the following commutation-anticommutation relations:

$$\{c_{\bar{k}x}, c_{\bar{k}'x}^{\dagger}\} = \delta_{\bar{k}\bar{k}'}, \quad \{c_d, c_d^{\dagger}\} = 1, \tag{43}$$

$$\{c_d, c_{\bar{k}x}^{\dagger}\} = \{c_d, c_{\bar{k}x}\} = 0, \qquad (44)$$

$$[c_d, \hat{\mathcal{N}}_s] = c_d, \tag{45}$$

which follow directly from the properties of  $\varphi_x$  and Eqs. (36). Note that  $c_d$  lowers the impurity spin, raises the total electron spin  $\hat{\mathcal{N}}_s$  and hence conserves the total spin  $S_T$ , whereas  $\psi_x$  conserves each of the impurity, electron and total spins.

To relate the number operator for the new *x*-pseudofermions to the quantum number  $\mathcal{N}_x$ , we must define a free reference ground state, say  $|0\rangle_{\mathcal{S}_{ext}}$ , in the extended subspace  $\mathcal{S}_{ext}$ , with respect to which the number of pseudo-fermions are counted. In analogy to Eq. (2), we define it by

$$c_{\bar{k}x}|0\rangle_{\mathcal{S}_{ext}} \equiv 0 \quad \text{for } \bar{k} > 0,$$
 (46a)

$$c_{\bar{k}x}^{\dagger}|0\rangle_{\mathcal{S}_{\text{ext}}} \equiv 0 \quad \text{for } \bar{k} \leq 0,$$
 (46b)

$$c_d |0\rangle_{\mathcal{S}_{\text{ext}}} \equiv 0 \quad \text{for } \varepsilon_d > 0, \text{ i.e., } n_d^{(0)} \equiv 0,$$
 (46c)

$$c_d^{\dagger}|0\rangle_{\mathcal{S}_{\text{ext}}} \equiv 0 \quad \text{for } \varepsilon_d \leq 0, \text{ i.e., } n_d^{(0)} \equiv 1.$$
 (46d)

Here  $\varepsilon_d$ , whose value will be derived below [see Eq. (52)], is the energy of the  $c_d$  pseudofermion, and  $n_d^{(0)}$  denotes its occupation number in the reference ground state  $|0\rangle_{S_{\text{ext}}}$ . Using colons to henceforth denote normal ordering of the pseudofermions with respect to  $|0\rangle_{S_{\text{ext}}}$ , we have  $:c_d^{\dagger}c_d$ :  $=c_d^{\dagger}c_d - n_d^{(0)}$ . Furthermore, we define the number operator for the *x* pseudofermions by  $\hat{N}_x \equiv \Sigma_{\bar{k}}: c_{\bar{k}x}^{\dagger}c_{\bar{k}x}:$  Then

$$\hat{N}_x = \hat{\mathcal{N}}_x - P/2 \tag{47}$$

holds as an operator identity. This can be seen intuitively by noting that  $\psi_x \sim \mathcal{F}_x \sim c_{\bar{k}x}$  [by Eq. (41)], hence the application of  $\psi_x$  (or  $\psi_x^{\dagger}$ ) to a state decreases (or increases) both  $\mathcal{N}_x$  and  $\bar{N}_x$  by one. These two numbers can thus differ only by a constant, which must ensure that  $\bar{N}_x$  is an integer. Our definition (46) of  $|0\rangle_{\mathcal{S}_{ext}}$  effectively fixes this constant to be P/2, by setting  $\bar{N}_x = 0$  for  $\mathcal{N}_x = P/2$  (see Appendix A 3 for a rigorous argument<sup>37</sup>).

We are now ready to refermionize the Hamiltonian H'. The kinetic energy of the  $\bar{k}$  pseudofermions obeys

$$\sum_{\bar{k}} \bar{k}: c_{\bar{k}x}^{\dagger} c_{\bar{k}x} := \frac{\Delta_L}{2} \hat{\bar{N}}_x (\hat{\bar{N}}_x + P) + \sum_q q b_{qx}^{\dagger} b_{qx}, \quad (48)$$

an operator identity which follows by analogy with Eqs. (1) and (18) (also see<sup>37</sup> Appendix A 3). Now note that  $\hat{N}_x(\hat{N}_x + P) = \hat{N}_x^2 - P/4$ , i.e., Eq. (48) does *not* contain a term linear in  $\hat{N}_x$ . Actually, the choice of the phase  $e^{-i(\hat{N}_x - 1/2)2\pi x/L}$  in our refermionization ansatz (41a) for  $\psi_x(x)$  was made specifically to achieve this. Hence Eq. (48) can be directly used to represent the kinetic energy of the *x* sector in Eq. (25) in terms of  $c_{\bar{k}x}$  fermions:

PRB 61

$$H_{x0} = \Delta_L \hat{\mathcal{N}}_x^2 / 2 + \sum_{q>0} q b_{qx}^{\dagger} b_{qx}$$
(49a)

$$=\sum_{\bar{k}} \bar{k}: c^{\dagger}_{\bar{k}x} c_{\bar{k}x}: +\Delta_L P/8.$$
(49b)

As a check, note that this equation also follows from the following observations. First, the equation of motion for the field  $\psi_x(x)$ , expressed as Eq. (41a) or (41b), is the same when calculated using Eq. (49a) or (49b), respectively, and therefore the latter two expressions can differ only by a constant; and secondly, this constant can be determined to be  $\Delta_L P/8$ , by requiring the free ground state energies for  $|0\rangle_{S_{ext}}$  given by the two expressions to be the same.

Finally, in the subspace  $S_{\text{phys}}$  [of Eq. (23)] and hence also in  $S_{\text{ext}}$ , we can use Eqs. (21) and (40) to express  $\hat{\mathcal{N}}_s S_z$  and  $\hat{\mathcal{N}}_s^2$  in terms of  $c_d^{\dagger} c_d$ . Thus, the EK-transformed 2CK Hamiltonian of Eqs. (33) and (34) takes the form

$$H' = H_{csf} + H_x + E_G + \text{const}, \tag{50}$$

$$H_{csf} = \sum_{c,s,f} \sum_{q>0} q b^{\dagger}_{qy} b_{qy}, \qquad (51)$$

$$H_{x} = \varepsilon_{d} : c_{d}^{\dagger} c_{d} : + \sum_{\bar{k}} \bar{k} : c_{\bar{k}x}^{\dagger} c_{\bar{k}x} :$$
$$+ \sqrt{\Delta_{L} \Gamma} \sum_{\bar{k}} (c_{\bar{k}x}^{\dagger} + c_{\bar{k}x}) (c_{d} - c_{d}^{\dagger}), \qquad (52)$$

$$E_{G} = \Delta_{L} [\mathcal{N}_{c}(1-P_{0}) + (\mathcal{N}_{c}^{2} + \mathcal{N}_{f}^{2} + S_{T}^{2} - 1/4)/2 + P/8] + \varepsilon_{d}(n_{d}^{(0)} - 1/2) + S_{T}h_{e}.$$
(53)

The charge, spin, and flavor degrees of freedom in  $H_{csf}$  evidently decouple completely.  $H_x$  in Eq. (52) has the form of a quadratic resonant level model whose "resonant level" has energy  $\varepsilon_d$  and width  $\Gamma$ , where  $\varepsilon_d \equiv h_i - h_e$  is the energy cost for an impurity spin-flip, and  $\Gamma \equiv \lambda_{\perp}^2/4a$ , which will be identified below as the Kondo temperature.

 $E_G$  is the "free ground state energy" of the subspace  $S_{\text{ext}}$ in the presence of magnetic fields. Its  $S_T h_{\rho}$  term implies that the magnetic fields do *not* enter only in the combination  $h_i$  $-h_{e}$  of  $\varepsilon_{d}$ , thus the role of the magnetic field  $h_{e}$  applied to the conduction electrons is somewhat different from that of the local field  $h_i$ . Note though, that for  $h_e = 2n\Delta_L$  (with n  $\in \mathbb{Z}$ ) the  $S_T h_e$  term can formally be absorbed (up to a total energy shift) by introducing a "new total spin"  $S'_T = S_T$ +2n, since then  $\Delta_L S_T^2/2 + S_T h_e = \Delta_L S_T'^2/2 - 2n^2 \Delta_L$ . Now, since the construction of the complete finite-size spectrum involves enumerating all possible values of  $S_T$ , and since the generalized gluing condition (69) to be derived below is invariant under  $S_T \rightarrow S_T + 2n$ , the finite-size spectrum for  $h_e$  $=2n\Delta_L$  and a local field  $h_i$  (so that  $\varepsilon_d = h_i - 2n\Delta_L$ ) will be identical to that for  $h_e = 0$  and a local field of  $h_i - 2n\Delta_L$  (so that  $\varepsilon_d$  is unchanged). The origin of this "periodicity" is that as  $h_e$  increases, at each value  $2n\Delta_L$  a "level crossing" occurs in which the free-electron ground state changes from, say,  $|\mathcal{N}_c, \mathcal{N}_s, \mathcal{N}_f, \mathcal{N}_x\rangle_0$  to a new one differing from it *only* in

the spin quantum number, namely,  $|\mathcal{N}_c, \mathcal{N}_s - 2, \mathcal{N}_f, \mathcal{N}_x\rangle_0$ , by flipping the topmost spin- $\uparrow$  electrons in both channels j = 1,2 to  $\downarrow$ .

For general values  $h_e \neq 2n\Delta_L$ , there is no such symmetry (essentially since electron-hole symmetry in the spin sector is lost), and the corresponding finite-size spectrum differs from that at the periodicity points in that some additional splittings of states occur.<sup>39</sup> For simplicity we henceforth set  $h_e=0$  and consider only a local magnetic field, with  $\varepsilon_d \equiv h_i$ , but the more general case  $h_e \neq 0$  can be treated completely analogously.

## V. FINITE-SIZE SPECTRUM OF 2CK MODEL

## A. Diagonalization of $H_x$

Since  $H_{csf}$  is trivial, we just have to diagonalize the resonant level part  $H_x$  in the extended subspace  $S_{ext}(S_T, \mathcal{N}_c, \mathcal{N}_f)$ , which is straightforward in principle, since  $H_x$  is quadratic. However, special care is needed regarding normal ordering: the change in ground state energy due to the interaction turns out to be of order  $-\Gamma$ , and the subleading (state-dependent) contributions of order  $\Delta_L$  relative to this energy have to be extracted carefully when constructing the finite-size spectrum.

As first step, we define new fermionic excitations, whose energies are strictly non-negative,

$$\begin{array}{l} \chi_{\overline{k}} \equiv (c_{\overline{k}x} + c_{-\overline{k}x}^{\dagger})/\sqrt{2} \\ \eta_{\overline{k}} \equiv -i(c_{\overline{k}x} - c_{-\overline{k}x}^{\dagger})/\sqrt{2} \end{array} \right\} \quad \text{for } \overline{k} > 0, \qquad (54a)$$

$$\alpha_0 \equiv c_{0x}^{\dagger} \quad \text{for } \ \overline{k} = 0 \text{ if } P = 1, \tag{54b}$$

$$\alpha_d \equiv \begin{cases} c_d & \text{for } \varepsilon_d > 0, \\ c_d^{\dagger} & \text{for } \varepsilon_d \le 0, \end{cases}$$
(54c)

where the  $\beta_{\bar{k}}$ 's decouple completely from the impurity:

$$H_{x} = \sum_{\bar{k} \ge 0} \bar{k} \alpha_{\bar{k}}^{\dagger} \alpha_{\bar{k}} + \sum_{\bar{k} > 0} \bar{k} \beta_{\bar{k}}^{\dagger} \beta_{\bar{k}} + |\varepsilon_{d}| \alpha_{d}^{\dagger} \alpha_{d}$$
$$+ \sum_{\bar{k} \ge 0} V_{\bar{k}} (\alpha_{\bar{k}}^{\dagger} + \alpha_{\bar{k}}) (\alpha_{d} - \alpha_{d}^{\dagger}).$$
(55)

Here the possible  $\overline{k}$  values are given by Eq. (42), and the hybridization amplitudes  $V_{\overline{k}}$  by

$$V_0 \equiv V_{\bar{k}\neq 0} / \sqrt{2} \equiv e^{i \pi n_d^{(0)}} \sqrt{\Gamma \Delta_L}.$$
(56)

Note that in Eq. (54) we purposefully defined  $\alpha_n^{\dagger}$  and  $\beta_{\bar{k}}^{\dagger}$ such that the free reference ground state  $|0\rangle_{S_{\text{ext}}}$ , by Eq. (46), contains *no*  $\alpha_n^{\dagger}$  or  $\beta_{\bar{k}}^{\dagger}$  excitations, i.e.,  $\alpha_d |0\rangle_{S_{\text{ext}}} = \alpha_{\bar{k}} |0\rangle_{S_{\text{ext}}}$  $= \beta_{\bar{k}} |0\rangle_{S_{\text{ext}}} = 0$ . Note too that  $\alpha_d^{\dagger} |0\rangle_{S_{\text{ext}}}$  is degenerate with  $|0\rangle_{S_{\text{ext}}}$  if  $\varepsilon_d = 0$ , as is  $\alpha_0^{\dagger} |0\rangle_{S_{\text{ext}}}$  in the odd electron sector, *P* = 1. (Figure 5 of Appendix C 5 illustrates these facts.)

Since the Hamiltonian Eq. (55) is quadratic, it can be diagonalized by a Bogoliubov transformation

$$H_{x} = \sum_{\bar{k}>0} \bar{k} \beta_{\bar{k}}^{\dagger} \beta_{\bar{k}} + \sum_{\varepsilon \ge 0} \varepsilon \, \tilde{\alpha}_{\varepsilon}^{\dagger} \tilde{\alpha}_{\varepsilon} + \delta E_{G} \,, \tag{57}$$

$$\widetilde{\alpha}_{\varepsilon}^{\dagger} = \sum_{n \in \{\overline{k}, d\}} \sum_{\nu = \pm} B_{\varepsilon n \nu} (\alpha_n^{\dagger} + \nu \alpha_n) / 2, \qquad (58)$$

where  $\delta E_G$  denotes the ground state energy shift of the *interacting vacuum*  $|\tilde{0}\rangle_{S_{ext}}$ , defined as

$$\tilde{\alpha}_{\varepsilon} |\tilde{0}\rangle_{\mathcal{S}_{\text{ext}}} = \beta_{\bar{k}} |\tilde{0}\rangle_{\mathcal{S}_{\text{ext}}} \equiv 0.$$
(59)

The non-negative eigenenergies  $\varepsilon$  and the coefficients  $B_{\varepsilon n\nu}$  are determined from the usual relations

$$[H_{x}, \tilde{\alpha}_{\varepsilon}^{\dagger}] = \varepsilon \, \tilde{\alpha}_{\varepsilon}^{\dagger}, \quad \{ \tilde{\alpha}_{\varepsilon}^{\dagger}, \tilde{\alpha}_{\varepsilon'} \} = \delta_{\varepsilon \varepsilon'}.$$
 (60)

These are solved explicitly in Appendix C,<sup>37</sup> with the following results. The excitation energies  $\varepsilon$  are the non-negative roots of the transcendental equation

$$\frac{\varepsilon 4 \, \pi \Gamma}{\varepsilon^2 - \varepsilon_d^2} = -\cot \, \pi (\varepsilon / \Delta_L - P/2), \tag{61}$$

and the ground state energy shift is

$$\delta E_G = \frac{|\varepsilon_d|}{2} + \sum_{\bar{k} \ge 0} \frac{\bar{k}}{2} - \sum_{\varepsilon \ge 0} \frac{\varepsilon}{2}.$$
 (62)

For  $\varepsilon > 0$ , the coefficients  $B_{\varepsilon n\nu}$  are given by

$$B_{\varepsilon d+} = \varrho(\varepsilon) |\varepsilon_d|, \quad B_{\varepsilon d-} = \varrho(\varepsilon)\varepsilon, \tag{63a}$$

$$B_{\varepsilon\bar{k}+} = \varrho(\varepsilon) \frac{2V_{\bar{k}} \varepsilon^2}{\varepsilon^2 - \bar{k}^2}, \quad B_{\varepsilon\bar{k}-} = \varrho(\varepsilon) \frac{2V_{\bar{k}} \varepsilon\bar{k}}{\varepsilon^2 - \bar{k}^2}, \quad (63b)$$

where the normalization factor  $\varrho(\varepsilon)$  is

$$\varrho(\varepsilon) = \left[\frac{2\Delta_L \Gamma}{\frac{1}{4}(\varepsilon^2 - \varepsilon_d^2)^2 + \Delta_L \Gamma(\varepsilon^2 + \varepsilon_d^2) + 4\pi^2 \Gamma^2 \varepsilon^2}\right]^{1/2}.$$
(64)

For  $\varepsilon = 0$ , the coefficients  $B_{0n\nu}$  must be considered separately and are given in Appendix C 2 b.<sup>37</sup> Equations (51), (53), (57), and (61)–(64), together with the gluing conditions (69) discussed in the next subsection, constitute a complete, analytic solution of the 2CK model along the EK line.

## **B.** Evolution of excitation energies

The eigenvalue equation (61) is a central ingredient of our analytical solution, since it yields the exact excitation energies  $\varepsilon$  of  $H_x$ , and also allows one to explicitly identify the various crossover scales of the problem. Let the label  $j = 0, 1, 2, \ldots$ , enumerate, in increasing order, the solutions  $\varepsilon_{j,P}$  of Eq. (61) in a sector with parity *P*. Their smooth evolution as functions of  $\Gamma$  and  $|\varepsilon_d|$  can readily be understood by a graphical analysis of Eq. (61), and is shown in Figs. 2(a) and 2(b) for P=0 and 1, respectively. All but the lowest-lying j=0 solutions can be parametrized as

$$\varepsilon_{j,P} = \Delta_L \left[ j - \frac{1}{2} - \frac{P}{2} + \delta_{j,P} \right], \quad j = 1, 2, 3, \dots, \quad (65a)$$

where  $\delta_{j,P} \in [0,1]$  is the shift of  $\varepsilon_{j,P}/\Delta_L$  from its  $\Gamma = \varepsilon_d$ =0 value and is determined self-consistently by



FIG. 2. Evolution of the excitation energies  $\varepsilon_{j,P}$ , found by numerically solving the eigenvalue equation (61). On the left the evolution is shown as function of  $\Gamma/\Delta_L \in [0,\infty)$  at  $T_h=0$ , and on the right as function of  $T_h/\Delta_L \in [0,\infty)$  at fixed  $\Gamma/\Delta_L \ge 1$ , for (a) P = 0 and (b) P = 1. These excitation energies are combined in Table II with excitations in the charge, spin, and flavor sectors to obtain the evolution of the full finite-size spectrum shown in Fig. 3.

$$\delta_{j,P} = \frac{1}{2} + \frac{1}{\pi} \arctan \frac{1}{4\pi} \left[ \frac{T_h}{\varepsilon_{j,P}} - \frac{\varepsilon_{j,P}}{\Gamma} \right], \quad (65b)$$

with  $T_h \equiv \varepsilon_d^2 / \Gamma$ . The lowest-lying modes are given by

$$\frac{\varepsilon_{0,0}}{\Delta_L} = \begin{cases} 0 & \text{for } \varepsilon_d = 0, \\ (-1/2 + \delta_{0,0}) \in (0, 1/2] & \text{for } \varepsilon_d \neq 0, \end{cases}$$
(66a)

$$\varepsilon_{0,1} = 0$$
 for all  $\Gamma, \varepsilon_d$  (66b)

(see also Appendix<sup>37</sup> C 2 b).

Equation (65b) shows very nicely that  $\Gamma$  and  $T_h$  are crossover scales: First, in the absence of magnetic fields, i.e., for  $|\varepsilon_d| = |h_i| = T_h = 0$ , the spectral regime below  $\Gamma$  is strongly perturbed  $[\delta_{j,P} \approx 1/2 \text{ for } \varepsilon_{j,P} \ll \Gamma]$ , whereas above  $\Gamma$  it is only weakly perturbed  $[\delta_{j,P} \approx 0 \text{ for } \varepsilon_{j,P} \gg \Gamma]$ . It is thus natural to identify the crossover scale  $\Gamma$  with the Kondo temperature  $T_K \approx \Gamma$ .

Secondly, in the presence of a local magnetic field,  $T_h = h_i^2/\Gamma > 0$  furnishes another crossover scale. When considering the  $T_h$ -induced shifts in  $\delta_{j,P}$  relative to their values for  $T_h = 0$ , several cases can be distinguished: (i) For  $T_h \ll \Delta_L$ , i.e., for  $|h_i|$  much smaller than a crossover field  $h_c \sim \sqrt{\Gamma}\Delta_L$ , none of the  $T_h$ -induced shifts are strong. (ii) For  $T_h \gg \Delta_L$ ,  $\Gamma$ , the crossover scale  $T_h$  divides the spectrum into two parts: the  $T_h$ -induced shifts are weak for all levels with  $\varepsilon \gg T_h$ , but strong for all those with  $\varepsilon \ll T_h$ . (iii) For  $\Gamma \gg T_h \gg \Delta_L$  one can distinguish three physically different regimes: the spectrum is NFL-like (nonuniform level spacings) in the intermediate regime  $T_h \ll \varepsilon \ll \Gamma$ , and Fermi-liquid-like (with uniform level spacing) in the extreme regimes  $\varepsilon \gg \Gamma$ 

6926

6927

and  $\varepsilon \ll T_h$ . In the last of these regimes (rightmost part of Fig. 2), the set of lowest-lying  $\varepsilon$ 's is identical to that for the *free* case  $T_h = 0$ ,  $\Gamma = 0$  (leftmost part of Fig. 2), except that the free case has one more  $\varepsilon = 0$  mode, reflecting the impurity's twofold degeneracy due to spin reversal symmetry for  $|h_i| = 0$ . Since at a finite temperature physical quantities are governed mostly by excitations of energy  $\varepsilon \sim T$ , they will show NFL behavior for  $\Gamma \gg T \gg T_h$  and Fermi liquid behavior for  $T \gg \Gamma$  or  $T \ll T_h$ .<sup>2,19,26,40</sup>

## C. Generalized gluing conditions

Next, we clarify how the exact many-body eigenstates of the full Hamiltonian are to be constructed from the various excitations in the c, s, f, and x sectors. A general eigenstate of  $H_{csf}+H_x$  in  $S_{ext}$  has the form

$$|\tilde{E}\rangle \propto \prod_{i=1}^{\mathcal{N}_{\tilde{a}}} \tilde{\alpha}_{\varepsilon_{i}}^{\dagger} \prod_{j=1}^{\mathcal{N}_{\beta}} \beta_{\tilde{k}_{j}}^{\dagger} |\tilde{0}\rangle_{\mathcal{S}_{\text{ext}}}, \qquad (67)$$

where the proportionality sign indicates that excitations in the c, s, and f sectors are not shown explicitly. However, as emphasized earlier, of all such states only those in the physical subspace  $S_{phys}$  must be retained, and all others discarded as being unphysical. To identify which  $|\tilde{E}\rangle$  are physical, we now derive a generalized gluing condition satisfied by them that relates the parity of the number of  $\tilde{\alpha}_{\varepsilon}^{\dagger}$  and  $\beta_{\bar{k}}^{\dagger}$  excitations in  $|\tilde{E}\rangle$  to its quantum numbers  $\mathcal{N}_c$ ,  $\mathcal{N}_f$ , and  $S_T$  in the c, f, and s sectors. To this end, we note that  $|\tilde{E}\rangle$  can be physical only if the state  $|E\rangle \equiv \lim_{\Gamma \to 0} |\tilde{E}\rangle$ , to which it reduces when  $\Gamma$ is adiabatically switched off, satisfies the free gluing conditions (20). The key to the derivation is the fact that although the hybridization interaction  $H'_{\perp}$  of Eq. (39) does not conserve the number of  $\alpha_n^{\dagger}$  excitations, it does conserve the parity of their number.

To be explicit, let  $\mathcal{P}_{\tilde{E}}$  be the the parity of the number of excitations of  $|\tilde{E}\rangle$  relative to  $|\tilde{0}\rangle_{S_{av}}$ :

$$\mathcal{P}_{\tilde{E}} = \langle \tilde{E} | \left[ \sum_{\varepsilon \ge 0} \tilde{\alpha}_{\varepsilon}^{\dagger} \tilde{\alpha}_{\varepsilon} + \sum_{\bar{k} > 0} \beta_{\bar{k}}^{\dagger} \beta_{\bar{k}} \right] \mod 2 | \tilde{E} \rangle.$$
(68)

During the adiabatic switch-off of  $\Gamma$ , this quantity of course remains *fixed*, and hence equals  $\mathcal{P}_{\tilde{E}}(\Gamma \rightarrow 0)$ . This in turn can be written as

$$\mathcal{P}_{\overline{E}}(\Gamma \to 0) = \langle E | \left[ \sum_{n=d,\overline{k} \ge 0} \alpha_n^{\dagger} \alpha_n + \sum_{\overline{k} \ge 0} \beta_{\overline{k}}^{\dagger} \beta_{\overline{k}} \right] \mod 2 | E \rangle$$
$$= \langle E | \left[ \hat{N}_x + \alpha_d^{\dagger} \alpha_d \right] \mod 2 | E \rangle$$
$$= \langle E | \left[ \left( \hat{\mathcal{N}}_x - \frac{P}{2} \right) + \hat{\mathcal{N}}_s - S_T - \frac{1}{2} + n_d^{(0)} \right] \mod 2 | E \rangle.$$

The first equation follows because the hybridization interaction preserves the parity of the excitation numbers; the second follows because the  $c_{\bar{k}x}^{\dagger}$  excitations counted by  $\hat{\mathcal{N}}_x$  are linear combinations of  $\alpha_{\bar{k}}$ ,  $\alpha_{\bar{k}}^{\dagger}$ ,  $\beta_{\bar{k}}$ , and  $\beta_{\bar{k}}^{\dagger}$ ; and the third follows from Eq. (47) for  $\hat{\mathcal{N}}_x$  and Eqs. (54c), (40), and (21) for  $\alpha_d$ . Imposing now the condition that  $|E\rangle$  must be in  $S_{\text{phys}}$  and hence satisfy Eq. (20b), we obtain

$$\mathcal{P}_{\widetilde{E}} = \begin{cases} [\mathcal{N}_c + \mathcal{N}_f - S_T - (P+1)/2] \mod 2 & (\varepsilon_d > 0), \\ [\mathcal{N}_c + \mathcal{N}_f - S_T - (P-1)/2] \mod 2 & (\varepsilon_d \leq 0). \end{cases}$$
(69)

This generalized gluing condition specifies which of all the possible states in  $S_{\text{ext}}$  are physical, i.e., are in  $S_{\text{phys}}$ ; it supplements the free gluing condition (20a), which stipulates that  $S_T \pm 1/2$  must be integer (half-integer) if  $\mathcal{N}_c$  and  $\mathcal{N}_f$  are integer (half-integer).

## D. Ground state energy shift

The form of Eq. (62) for the change in ground state energy  $\delta E_G$  suggests that it can be interpreted as *the dynamical binding energy of the impurity spin*, which results from the impurity-induced energy shifts of all the states in the filled Fermi sea. [The factor 1/2 in Eq. (62) reflects the fact<sup>2,41</sup> that only "half" of the *x*-pseudofermion field, namely,  $\psi_x + \psi_x^{\dagger}$ , couples to the impurity in Eq. (39), while  $\psi_x - \psi_x^{\dagger}$  remains free.] For  $\varepsilon_d = 0$ , the number of levels strongly shifted by the interaction is [by Eq. (65b)] of order  $\Gamma/\Delta_L$ , and each of these gets shifted roughly by  $\Delta_L/2$ ; we can thus estimate that the binding energy  $|\delta E_G|$  will be of order  $\Gamma \sim T_K$ .

However, since the level shifts  $\Delta_L \delta_{j,P}$  also have a *P*-dependence of order  $\sim \Delta_L^2/\Gamma$  [from Eq. (65b)], the total ground state energy shift  $\delta E_G$  will have a *P* dependence too, of order  $\sim \Delta_L$ . We therefore write

$$\delta E_G \equiv \delta E_G^0 + P \ \delta E_G^P, \tag{70}$$

where the first term is *P* independent and hence gives only an overall energy shift. In contrast,  $\delta E_G^P$  affects the finite-size spectrum since it shifts the odd electron states (*P*=1) relative to even electron states (*P*=0), and hence must be evaluated with particular care. This is done in Appendix C4,<sup>37</sup> where we find, for  $\Gamma/\Delta_L \ge 1$ ,

$$\delta E_G^P = \begin{cases} -\Delta_L / 8 & (T_h = 0), \\ 0 & (T_h \gg \Delta_L), \end{cases}$$
(71)

$$\delta E_G^0 \approx \begin{cases} -2\Gamma[\ln(D/4\pi\Gamma)+1] & (T_h=0), \\ -2\Gamma[\ln(D/|\varepsilon_d|)+1] & (T_h \gg \Delta_L, \Gamma). \end{cases}$$
(72)

Here  $D \gg \Gamma$ ,  $T_h$  is a cutoff needed to regularize the sums in Eq. (62). Note that for  $T_h = 0$ , Eq. (72) is consistent with the estimate for  $\delta E_G$  above, since  $D \approx 1/a$  and  $\Gamma = \lambda_{\perp}^2/4a$ . For  $T_h \gg \Gamma$ , the magnetic field  $|\varepsilon_d|$  takes over as lower energy scale in the logarithm instead of  $\Gamma$ .

## E. Construction of the finite-size spectrum

Now we are finally ready to construct the finite-size many-body excitation spectrum of the 2CK model. In doing so, we shall generally use calligraphic  $\mathcal{E}$ 's to denote dimensionless energies measured in units of  $\Delta_L$ . Specifically, we shall construct the dimensionless energies

$$\widetilde{\mathcal{E}}(L) = [\widetilde{E}(L) - \widetilde{E}_{\min}(L)] / \Delta_L, \qquad (73)$$



FIG. 3. Evolution of the many-body finite-size spectrum of the 2CK model, for antiperiodic boundary conditions  $(P_0=1)$ , from the free Fermi-liquid fixed point to the NFL fixed point, and the additional crossover induced by a local magnetic field to a phaseshifted Fermi-liquid fixed point. All eigenstates of H' of Eq. (50) are shown for which  $\mathcal{E}_{NFL} \leq 1$ , as well as some higher-lying states, with degeneracies given in brackets (in Ref. 4, the degeneracies for  $\mathcal{E}_{\text{NFL}} = 1$  were incorrect). (a) When  $\lambda_z$  is tuned from 0 to its Emery-Kivelson value  $\lambda_z = 1$ , with  $\lambda_{\perp} = \varepsilon_d = 0$ , the free Fermi-liquid spectrum  $\mathcal{E}_{\text{free}}$  at  $\lambda_z = 0$  evolves smoothly into a simple phase-shifted spectrum  $\mathcal{E}_{\text{phase}}$  at  $\lambda_z = 1$ . (b) When  $\Gamma/\Delta_L = \lambda_{\perp}^2/(4a\Delta_L)$  is tuned from 0 to  $\infty$  along the EK line, i.e., with  $\lambda_z = 1$  and  $\varepsilon_d = 0$ , the spectrum crosses over from  $\mathcal{E}_{\text{phase}}$  to the non-Fermi-liquid spectrum  $\mathcal{E}_{\text{NFL}}$  at  $\Gamma/\Delta_L = \infty$ , which agrees with NRG and CFT results. (c) Turning on a local magnetic field  $\varepsilon_d = h_i$  (with  $h_e = 0$ ) by tuning  $|\varepsilon_d|/\Gamma$  from 0 to  $\infty$  with  $\lambda_z = 1$ ,  $\Gamma \gg \Delta_L$  fixed, then induces a further crossover from  $\mathcal{E}_{NFL}$  to  $\mathcal{E}_{ph}.$  For the lowest levels this crossover occurs when  $|\varepsilon_d|/\Gamma \gtrsim 1$ , since then the crossover parameter used in Fig. 2, namely,  $T_h/\Delta_L = (\varepsilon_d/\Gamma)^2 (\Gamma/\Delta_L)$ , is  $\ge 1$ . The  $\mathcal{E}_{ph}$  spectrum is identical to the phase-shifted spectrum  $\mathcal{E}_{phase}$  of  $\lambda_z = 1$  and  $\lambda_\perp$  $=\varepsilon_d=0$ , apart from a degeneracy factor of 2 due to the lack of spin reversal symmetry.

associated with the lowest few exact many-body eigenstates  $|\tilde{E}\rangle$  of the full Hamiltonian H' of (50), measured relative to its ground state energy  $\tilde{E}_{\min}$ . For the sake of simplicity we only consider the case with periodicity index  $P_0=1$  [see Eq. (3)], for which the  $\psi_{\alpha j}$ 's have anti-periodic boundary conditions. In this case the free ground state in the electronic sector is unique, namely,  $|\tilde{0}\rangle_0$ , which somewhat simplifies the counting of states. (Of course, one can use the same procedure for  $P_0=0$ , with similar results.)

The construction proceeds in three steps: we first evolve toward the EK line, second evolve along the EK line, and third turn on a local magnetic field. The results are summarized in Fig. 3 and Table I. For technical details of the con-

TABLE I. Summary of the finite-size spectrum of Fig. 3 for the 2CK model, at the four points  $\lambda_z = \lambda_\perp = \varepsilon_d = 0$  ( $\mathcal{E}_{\text{free}}$ );  $\lambda_z = 1$ ,  $\lambda_\perp = \varepsilon_d = 0$  ( $\mathcal{E}_{\text{phase}}$ );  $\lambda_z = 1$ ,  $\Gamma/\Delta_L = \infty$ ,  $\varepsilon_d = 0$  ( $\mathcal{E}_{\text{NFL}}$ ); and  $\lambda_z = 1$ ,  $\Gamma/\Delta_L = \infty$ ,  $\mathcal{T}_h/\Delta_L = \infty$  ( $\mathcal{E}_{\text{ph}}$ ). We list all energies  $\mathcal{E} \leq 1$  (in units of  $\Delta_L$ ) and give their total degeneracies in brackets.

2	£ free	$\mathcal{E}_{ ext{phase}}$	$\mathcal{E}_{ m NFL}$	$\mathcal{E}_{ m ph}$
0	(2)	0 (2)	0 (2)	0 (1)
1/2	(16)	1/4 (8)	1/8 (4)	1/4 (4)
1	(54)	1/2 (12	) 1/2 (10)	1/2 (6)
		3/4 (16	) 5/8 (12)	3/4 (8)
		1 (34	) 1 (26)	1 (17)

struction, see Fig. 5 and Table II in Appendix C 5.<sup>37</sup> Here we just state the main ideas.

(i) *Phase-shifted spectrum.* For  $\lambda_z \in [0,1]$  at  $\lambda_{\perp} = \varepsilon_d = 0$ , the impurity has no dynamics, thus the spectrum is that of a *free-electron Fermi liquid with a S<sub>z</sub>-dependent phase shift in the spin sector*, given by  $H'(\lambda_{\perp}=0)$  of Eq. (33). It evolves linearly with increasing  $\lambda_z$ , from  $\mathcal{E}_{\text{free}}$  at  $\lambda_z = 0$  to  $\mathcal{E}_{\text{phase}}$  at  $\lambda_z = 1$ , see Fig. 3(a).

(ii) Crossover spectrum. Next we study the spectrum along the EK line for  $\Gamma/\Delta_L \in [0,\infty)$  at  $\lambda_z = 1$ ,  $\varepsilon_d = 0$ . To this end one first has to enumerate the lowest-lying physical eigenstates  $|\tilde{E}\rangle$  of the full Hamiltonian H' in terms of the excitations  $\tilde{\alpha}^{\dagger}_{\varepsilon_{j,P}}$ ,  $\beta^{\dagger}_{k}$  and  $b^{\dagger}_{qy}$  which diagonalize it, and follow the evolution with increasing  $\Gamma/\Delta_L$  of the excitation energies  $\varepsilon_{j,P}$  (shown in Fig. 2), and of the ground state energy shift  $\delta E^P_G$  [see Eq. (71)]. This yields the crossover shown in Fig. 3(b) from the phase-shifted to the NFL fixed point spectrum, consisting of a set of universal, dimensionless energies defined by

$$\mathcal{E}_{\text{NFL}} \equiv \lim_{L \to \infty} \frac{\tilde{E}(L; \varepsilon_d = 0, \Gamma) - \tilde{E}_{\min}(L; \varepsilon_d = 0, \Gamma)}{\Delta_L}.$$
 (74)

Satisfyingly, the spectrum of  $\mathcal{E}_{NFL}$  energies found in Fig. 3(b) and Table I (degeneracies are given in brackets) coincides obtained in with the ones NRG and CFT calculations.<sup>16,18,22,23</sup> This constitutes a direct and straightforward analytical proof of the soundness of the latter approaches. In particular, it proves<sup>42</sup> the so-called *fusion hypothesis* employed by Affleck and Ludwig in their CFT calculation of this spectrum.<sup>22,23</sup> As is well-known from CFT,<sup>43</sup> each of the fixed-point values  $\mathcal{E}_{NFL}$  can be associated with the scaling dimension of one of the operators characterizing the fixed point. The occurrence of  $\mathcal{E}_{NFL}$ 's that are not simply integers or half-integers is thus a very direct sign of NFL physics, since these correspond to nonfermionic operators.

Our NFL spectrum demonstrates explicitly that the spin anisotropy is irrelevant at the NFL fixed point,<sup>18</sup> since if we take the continuum limit  $\Delta_L \rightarrow 0$  at fixed  $\Gamma$ , the fixed point spectrum is evidently reached *independently* of the specific value of  $\Gamma$ . More formally: the symmetry of our anisotropic starting Hamiltonian with respect to transformations in the charge, spin and flavor sectors is  $U(1)_c \times U(1)_s \times SU(2)_f$ , i.e., in the spin sector it is only invariant under spin rotations around the z axis; in contrast, Affleck and Ludwig derived the NFL fixed point spectrum by assuming it to have the complete  $U(1)_c \times SU(2)_s \times SU(2)_f$  symmetry of the free model. The fact that the low-energy part ( $\varepsilon \ll T_K$ ) of our NFL fixed point spectrum coincides with theirs beautifully illustrates how the broken symmetry of the original model is restored in the vicinity of the NFL fixed point, and thus proves another central assumption of the CFT solution of the 2CK model, in agreement with the NRG study of Pang and Cox.<sup>17</sup>

The fact that the exact eigenenergies of H' interpolate smoothly between their values for  $\lambda_{\perp} = 0$  and  $\lambda_{\perp} \neq 0$  [Fig. 3(b)] may at first seem somewhat surprising, because a common way of heuristically characterizing a NFL is that its quasiparticles are orthogonal to the bare ones of the corresponding free Fermi liquid. This is referred to as the "breakdown of Landau's quasiparticle construction," since in Landau's picture of a Fermi liquid, the dressed quasiparticles and the corresponding bare ones have finite overlap. Here, in fact, one can readily check that  $_{S_{ext}}\langle \tilde{0} | \alpha_{\bar{k}} \tilde{\alpha}^{\dagger}_{\varepsilon(\bar{k})} | \tilde{0} \rangle_{S_{ext}}$  is nonzero [where  $\varepsilon(\bar{k})$  is the excitation energy that reduces to  $\bar{k}$  as  $\Gamma/\Delta_L \rightarrow 0$ ], implying that in the  $\alpha$ -basis the system *is* a Fermi liquid. However, this does not contradict the fact that in the *original*  $c_{k\alpha j}$  *basis* the system nevertheless behaves as a NFL, since the bosonization-refermionization relation between states in the  $\alpha_{\bar{k}}$  and  $c_{k\alpha j}$  bases is very highly nonlinear.

(iii) Crossover due to local magnetic field. Finally, we turn on a local magnetic field,  $\varepsilon_d = h_i \neq 0$  at fixed  $\lambda_z = 1$  and  $\Gamma/\Delta_L \ge 1$ , thus breaking spin reversal symmetry. The further evolution of the excitation energies  $\varepsilon_{i,P}$  as functions of increasing  $T_h/\Delta_L$ , shown in Fig. 2(b), yields the magneticfield-induced crossover, shown in Fig. 3(c), from the NFL fixed point energies  $\mathcal{E}_{\text{NFL}}$  to a set of energies  $\mathcal{E}_{\text{ph}}$  corresponding to a phase-shifted Fermi liquid fixed point. For  $T_h/\Delta_L$  $\gg$  1, the impurity level evidently becomes empty for all lowlying states,  $\langle c_d^{\dagger} c_d \rangle = 0$ , i.e., the impurity spin is frozen in the state  $S_z = \downarrow$ . Indeed, the spectrum  $\mathcal{E}_{ph}$  which one recovers is precisely the same phase-shifted spectrum as  $\mathcal{E}_{phase}$  at the point  $\lambda_z = 1$  and  $\lambda_\perp = 0$ , apart from a degeneracy factor of 2, due to the lack of spin reversal symmetry, compare Table I. This shows nicely how the magnetic field "erases" all traces of NFL physics for the lowest-lying part of the spectrum, since low-energy electrons cannot overcome the Zeeman energy cost for a spin flip in a magnetic field.

## F. Finite-size behavior of physical quantities

Let us now briefly discuss the finite-size, T=0 behavior of the entropy, susceptibility, and the fluctuations in  $\mathcal{N}_x$  at the NFL fixed point. The *entropy* of the ground state at T=0,  $\varepsilon_d$ =0 is evidently simply ln 2 for any *L*, since the ground state is twofold degenerate (see Fig. 3). This should be contrasted<sup>44</sup> with the famous result  $\frac{1}{2}$ ln 2 that one obtains<sup>23(c)</sup> taking the limit  $L \rightarrow \infty$  before  $T \rightarrow 0$ . The difference simply illustrates that the order of limits does not commute, since for finite *L* the system is always gapped.

The susceptibility at T=0 due to a local field  $h_i$  is defined by  $\chi = -\partial^2 \tilde{E}_G / \partial h_i^2$ . Since  $\tilde{E}_G = E_G + \delta E_G$ , we simply have to evaluate [by Eqs. (53), (62)] the sum  $\chi = \frac{1}{2} \Sigma_{\varepsilon} (\partial^2 \varepsilon / \partial h_i^2)$ . For  $h_i = 0$ , the summands can be determined by differentiating Eq. (61), giving

$$\chi(h_i=0) = \sum_{\varepsilon>0} \frac{1}{\varepsilon} \frac{4\pi\Gamma\Delta_L}{\{\Delta_L 4\pi\Gamma + \pi[(4\pi\Gamma)^2 + \varepsilon^2]\}}$$
(75)

$$\approx \frac{1}{4\pi^2\Gamma} \ln(4\pi\Gamma/\Delta_L) \quad \text{(for } \Gamma \gg \Delta_L\text{)}.$$
(76)

The fact that  $\chi(h_i=0) \rightarrow \infty$  as  $L \rightarrow \infty$  is of course a characteristic sign of 2CK NFL physics: it illustrates the instability of the NFL phase with respect to a local symmetry

breaking.<sup>40</sup> At finite temperatures *T* takes over the role of the infrared cutoff  $\Delta_L$ , so that the susceptibility diverges logarithmically with *T*.<sup>19,2</sup>

The fluctuations in  $\hat{\mathcal{N}}_x$  can be quantified by calculating  $\langle \hat{\mathcal{N}}_x^2 \rangle - \langle \hat{\mathcal{N}}_x \rangle^2$ . In Appendix C 6 this is done at  $\varepsilon_d = 0$  for the physical ground state of  $\mathcal{S}_{phys}$  for both P = 0 and  $1.^{37}$  We find that  $\langle \hat{\mathcal{N}}_x \rangle = 0$  for arbitrary ratios of  $\Gamma/\Delta_L$ , showing that the ground state contains equal amounts of spin from both flavors j = 1,2, as expected from the 2CK model's flavor symmetry. Furthermore,  $\langle \hat{\mathcal{N}}_x^2 \rangle = P/4$  for  $\Gamma/\Delta \rightarrow 0$ , as expected intuitively, since in this limit the considered ground states are linear combinations of states with  $\mathcal{N}_x = \pm P/2$ . In contrast, in the limit  $\Gamma/\Delta_L \ge 1$ , the fluctuations diverge logarithmically with system size,  $\langle \hat{\mathcal{N}}_x^2 \rangle \approx (1/\pi^2) \ln \Gamma L$ , illustrating how strongly the impurity perturbs the Fermi sea at the NFL fixed point.

#### VI. RELATION TO VARIOUS RG METHODS

In the literature several RG methods have been applied to the multichannel Kondo model. In this section we relate these to our finite-size bosonization technique, by showing how the strategies employed by them can be implemented, in an *exact way*, within the latter.

#### A. High-energy cutoff scaling techniques

The most common types of RGs are the ones used in particle physics and in the standard treatment of critical phenomena. In these RG procedures, one reduces a high-energy cutoff, say  $\tilde{D}$ , in order to gradually eliminate some high-energy degrees of freedom, arguing that they only slightly influence the low-energy physics of the system. The change in the cutoff must be compensated by rescaling the model's dimensionless coupling constants and masses in order to keep the physical properties (different inherent energy scales and dressed masses) invariant. These kinds of scaling procedures, which include Anderson's poor man's scaling,<sup>45</sup> the multiplicative RG,<sup>6</sup> and the Yuval-Anderson RG,<sup>46</sup> have been widely used in the continuum limit ( $L \rightarrow \infty$ ) to study the multichannel Kondo model.<sup>47,48,17,49</sup>

In our case the high-energy cutoff  $\tilde{D}$  can be identified with the cutoff 1/a of the boson fields  $\phi_{\alpha j}$ ,  $\tilde{D} \sim 1/a$ . Then the scaling dimension  $\gamma$  of an operator with dimensionless coupling  $\lambda$  can be determined from the scaling equation  $d \ln \lambda/d \ln \tilde{D} = -d \ln \lambda/d \ln a = \gamma(\lambda,...)$ , and the operator is relevant, marginal or irrelevant for  $\gamma < 0$ , = 0, or > 0, respectively.

Now, along the EK line one immediately obtains the scaling equations<sup>27</sup>

$$\frac{d\lambda_{\perp}}{d\ln a} = \frac{1}{2}\lambda_{\perp}, \quad \lambda_z \equiv 1.$$
(77)

The first, which follows from the requirement of the invariance of the Kondo scale  $\Gamma = \lambda_{\perp}^2/4a$ , shows that  $\lambda_{\perp}$  is relevant and grows under bandwidth rescaling, with dimension -1/2. As explained earlier, the second equation follows from the absence of the leading irrelevant operator at the EK line.

Equations (77) exactly coincide with the ones obtained with the Yuval-Anderson technique<sup>7</sup>

$$\frac{d\lambda_{\perp}}{d\ln a} = \left(4\frac{\delta}{\pi} - 8\frac{\delta^2}{\pi^2}\right)\lambda_{\perp}, \qquad (78a)$$

$$\frac{4}{\pi} \frac{d \,\delta}{d \ln a} = \left(1 - \frac{4 \,\delta}{\pi}\right) \lambda_{\perp}^2, \qquad (78b)$$

if in these the phase shift  $\delta = \lambda_z \pi/4$  is replaced by  $\pi/4$ , as appropriate for the EK line.<sup>17</sup>

In a finite local magnetic field  $\varepsilon_d = h_i$ , for energies below the scale  $T_h = h_i^2/\Gamma$ , the magnetic field destroys the non-Fermi-liquid behavior and a Fermi liquid is recovered. By requiring the invariance of  $T_h$  one immediately derives that, as long as the high-energy cutoff 1/a is much larger than the Kondo scale  $\Gamma$ , the field  $h_i$  must be invariant under the RG transformation

$$\frac{dh_i}{d\ln a} = 0 \quad (1/a \gg \Gamma). \tag{79}$$

However, once the cutoff is reduced sufficiently so that  $1/a \ll \Gamma$ , the role of  $\Gamma$  is taken over by 1/a, i.e.,  $T_h$  is now given by  $h_i^2 a$ , thus Eq. (79) must be replaced by

$$\frac{dh_i}{d\ln a} = -\frac{1}{2}h_i \quad (1/a \ll \Gamma).$$
(80)

To determine the dimension of the magnetic field one has to rewrite Eqs. (80) and (79) in terms of the *dimensionless* magnetic field,  $\tilde{h} \equiv h_i a$ . Then it immediately follows that close to the NFL fixed point the local field has dimension -1/2 while in the regime  $1/a \ge \Gamma$  its dimension is -1; it is therefore relevant in both cases.

Equations (79) and (80) are in complete agreement with those obtained by the Yuval-Anderson technique.<sup>7</sup> We remark at this point that perpendicular local magnetic fields  $h_{x,y}$  (i.e., perturbations of the form  $h_x S_x$  or  $h_y S_y$ ) are known<sup>7</sup> to scale differently from  $h_i = h_z$ , and at the EK line their scaling dimension is known to be -1/2 even in the region  $1/a \ge \Gamma$ .

#### B. Connection to numerical renormalization group

In this subsection we show that an analysis of our finitesize spectrum as function of L in fact represents an analytical version of Wilson's NRG.<sup>50</sup> In Wilson's procedure one divides the Fermi sea into energy shells using a logarithmic mesh characterized by a parameter  $\Lambda > 1$ , and then maps the model onto an equivalent one in which the impurity is coupled to the end of an infinite conducting chain, where the hopping between the sites *n* and n+1 scales as  $\Lambda^{-n/2}$ . The n'th site in this chain represents an "onion-skin" shell of conduction electrons, characterized by spatial extent  $\sim \Lambda^{n/2}$ around the impurity site and energy  $\sim \Lambda^{-n}$ . The NRG transformation is then defined by considering truncated chains of length N with Hamiltonian  $H_N$ , and consists of (i) adding a new site to the end of the chain  $H_N \rightarrow H_{N+1}$  and (ii) rescaling the new Hamiltonian by  $\Lambda: H_{N+1} \rightarrow \Lambda H_{N+1}$ . Trivially, step (i) reduces the mean level spacing by a factor of  $1/\Lambda$ , while step (ii) is needed to measure all energies in units of the new

PRB <u>61</u>

mean level spacing. This strategy is implemented by numerically diagonalizing  $H_{N+1}$  and retaining only the lowest few hundred levels. One finds that after a number of iterations the spectrum of  $H_N$  converges to a fixed, universal set of energies, characteristic of some fixed point Hamiltonian.<sup>17</sup> For the 2CK model this spectrum<sup>16</sup> is identical to the one obtained by boundary CFT.<sup>18</sup>

The NRG strategy can easily be interpreted in terms of our finite-size calculations. Step (i) corresponds to increasing the system size  $L \rightarrow \Lambda L$  (i.e., reducing the level spacing  $\Delta_L$  $\rightarrow \Delta_{\Lambda L} = \Delta_L / \Lambda$ ), while step (ii) is equivalent to measuring all energies in units of  $\Delta_{\Lambda L}$ . Combining both steps, an "analytical RG step" thus has the form

$$\frac{H_x(L,\Gamma,\varepsilon_d)}{\Delta_L} \to \frac{H_x(\Lambda L,\Gamma,\varepsilon_d)}{\Delta_{\Lambda L}} = \frac{H_x(L,\Lambda\Gamma,\Lambda\varepsilon_d)}{\Delta_L},$$
(81)

where the last equality follows identically from Eq. (52). For  $\varepsilon_d = 0$  this means that increasing the system size at fixed  $\Gamma$  is equivalent to increasing  $\Gamma$  at fixed *L*, emphasizing once more that in this case the spectrum depends only on  $\Gamma/\Delta_L$ . Therefore the "spectral flow" as function of  $\Gamma/\Delta_L$  in Fig. 3 can be viewed as the analytical version of an NRG spectrum as a function of iteration number.

The fact that changing the system size is equivalent to rescaling the couplings has actually been exploited in several NRG papers to construct the "exact" scaling trajectories in the space of the bare couplings: this can be done by rescaling the couplings after each NRG step in such a way that the NRG spectrum remains invariant, as in the seminal paper of Cragg, Lloyd, and Nozières,<sup>16</sup> or equivalently in such a way that the energy-dependent dynamical correlation functions remain invariant.<sup>51</sup>

#### C. Finite-size scaling

It is also straightforward to implement Wilson's prescription<sup>52</sup> for extracting the exact scaling exponent of a perturbation around the fixed point, say  $\delta \lambda \hat{O}$ , from its effect on the finite-size spectrum: In general, it causes the dimensionless energy  $\tilde{\mathcal{E}}(L)$  [of Eq. (73)] (calculated at a finite, nonzero  $\Delta_L \ll \Gamma$ ) to differ from its universal fixed point value  $\mathcal{E}_{\text{NFL}}$  [of Eq. (74)] by an amount  $\delta \tilde{\mathcal{E}}(L)$ , whose leading asymptotic behavior for  $L \rightarrow \infty$  is

$$\delta \tilde{\mathcal{E}}(L) \equiv \tilde{\mathcal{E}}(L) - \mathcal{E}_{\rm NFL} \sim (\delta \lambda / L^{\gamma})^n, \tag{82}$$

where  $n \ge 1$  is some integer and  $\gamma$  is the scaling dimension of the operator  $\hat{O}$ . Thus deviations from the universal spectrum are characteristic of the operator content of the fixed point.

We first consider the situation *on* the EK line (i.e., for  $\lambda_z=1$ ), and close to the NFL fixed point, where  $\Delta_L/\Gamma$  and  $T_h/\Delta_L$  are both  $\ll 1$  (*at* the NFL fixed point they are both 0). For  $j \ge 1$ , the leading deviations  $\varepsilon_{j,P}/\Delta_L - (\varepsilon_{j,P}/\Delta_L)_{\text{NFL}}$  of the dimensionless single-particle excitation eigenenergies from their NFL fixed point values are then given [from Eq. (65)] by

PRB 61

$$\delta_{j,P} - (\delta_{j,P})_{\rm NFL} = \frac{1}{4\pi^2} \left[ \frac{T_h}{\Delta_L(j - P/2)} - \frac{\Delta_L(j - P/2)}{\Gamma} \right].$$
(83)

The leading dependence on the local magnetic field via  $T_h/\Delta_L$  is evidently  $[h_i L^{1/2}]^2$ , which grows as  $L \rightarrow \infty$ . This shows that a local magnetic field has dimension  $\gamma_{h_i} = -1/2$  and is relevant: for an arbitrarily small  $h_i$ , there exists a system size *L* above which the lowest part of the spectrum and the ground state properties of the model are drastically affected, namely when  $\Delta_L \lesssim T_h$ , or equivalently,  $|h_i| > h_c = \sqrt{\Gamma \Delta_L}$ , where  $h_c$  denotes the crossover scale of section V B.

In the absence of magnetic fields, the leading term in Eq. (83) vanishes with increasing *L* as  $(\Gamma L)^{-1}$ , implying that the least irrelevant irrelevant operator *on* the EK line has dimension  $\gamma_{EK}=1$ . Thus, we conclude that the leading irrelevant operators with dimension  $\gamma=1/2$  that were found in the CFT treatment<sup>23(d)</sup> are absent *on* the EK line, in agreement with Refs. 2 and 26.

Now let us move away from the EK line by taking  $\lambda_z = 1 + \delta \lambda_z$ , and do perturbation theory in  $\delta \lambda_z$ , i.e., in  $\delta H'_z$  of Eq. (35). Then the operators with dimension  $\gamma = 1/2$  just mentioned immediately show up: As shown in detail in Appendix C 7,<sup>37</sup> we find that the "zero mode" term  $\delta \lambda_z \Delta_L \hat{\mathcal{N}}_s S_z$  of (35) (which does not occur in the continuum limit considered in Ref. 2), affects the spectrum already in first order in  $\delta \lambda_z$ : in the absence of magnetic fields, the first excited states (with  $\mathcal{E}_{NFL} = 1/8$ ) are shifted relative to the doubly degenerate ground states (with  $\mathcal{E}_{NFL} = 0$ ) by an amount

$$\delta \widetilde{\mathcal{E}}(L) \simeq -\frac{1}{4} \delta \lambda_z (1 + 4 \pi^2 \Gamma / \Delta_L)^{-1/2} \sim L^{-1/2}.$$
(84)

This implies that the leading operator that appears as one moves away from the EK line has dimension 1/2 and is irrelevant. Thus, the *EK line is stable against perturbations away from it.* 

In the presence of a local magnetic field  $\varepsilon_d = h_i$ , one finds in the continuum limit  $\Delta_L \ll \Gamma, h_i$  that the ground state degeneracy is split by an amount

$$\delta \widetilde{\mathcal{E}}(L) = \begin{cases} \frac{\delta \lambda_z}{2 \pi^2} \frac{|h_i|}{\Gamma} \ln \frac{|h_i|}{4 \pi \Gamma} & (\Delta_L \ll h_i \ll \Gamma), \\ \frac{\delta \lambda_z}{2} \left( 1 - \frac{4\Gamma}{|h_i|} \right) & (\Delta_L \ll \Gamma \ll h_i). \end{cases}$$
(85)

This shows that the magnetic-field behavior *along* the EK line is not completely generic, since it misses this part of the  $h_i$  dependence of the magnetic-field-induced crossover. Note that the  $|h_i|/\Gamma \ln|h_i|/\Gamma$  behavior that occurs for a local magnetic field of intermediate strength is consistent with the conclusions of the NRG studies of Ref. 18 for the  $h_i$ -dependence of a certain phase shift that can be used to characterize the NRG spectra.

Finally, we would like to comment here on the identification of the Kondo scale  $T_K$ . In Sec. V B we showed that the crossover scale below which the finite-size spectrum takes its fixed-point form (at  $h_i=0$ ) was  $\Gamma$ , and hence concluded that



FIG. 4. Evolution of the many-body finite-size spectrum of the 1CK model, for antiperiodic boundary conditions ( $P_0=1$ ), from the free Fermi-liquid fixed point to the strong-coupling Fermi-liquid fixed point. All eigenstates of H' of Eq. (D28) are shown for which  $\mathcal{E}_{FL} \leq 1$ , as well as some higher-lying states, with degeneracies given in brackets. (a) When  $\lambda_z$  is tuned from 0 to its Toulouse-point value  $\lambda_z^* = 2 - \sqrt{2}$ , with  $\lambda_{\perp} = \varepsilon_d = 0$ , the free Fermi-liquid spectrum  $\mathcal{E}_{free}$  at  $\lambda_z = 0$  evolves smoothly into a simple phase-shifted spectrum  $\mathcal{E}_{phase}$  at  $\lambda_z = \lambda_z^*$ . (b) When  $\Gamma/\Delta_L = \lambda_{\perp}^2/(4a\Delta_L)$  is tuned from 0 to  $\infty$  at the Toulouse point, i.e., with  $\lambda_z = \lambda_z^*$  and  $\varepsilon_d = 0$ , the spectrum crosses over from  $\mathcal{E}_{phase}$  to the strong-coupling Fermiliquid spectrum  $\mathcal{E}_{FL}$  at  $\Gamma/\Delta_L = \infty$ . The latter is identical to the free Fermi-liquid spectrum ( $\lambda_z = \lambda_{\perp} = \varepsilon_d = 0$ ) for periodic boundary conditions ( $P_0 = 0$ ), in agreement with Wilson's NRG results (Ref. 50).

 $T_K \simeq \Gamma$ . This differs from the suggestion of Sengupta and Georges<sup>26</sup> that the Kondo scale in the anisotropic 2CK model close to the EK line is not  $\Gamma$  but rather  $\Gamma/(\delta \lambda_z)^2$ . This scale emerged naturally in their calculation of the total susceptibility enhancement due to the impurity, which yielded  $\chi_{imp} \sim (\delta \lambda_z)^2/\Gamma \ln(\Gamma/T)$  (at  $h_i=0$ ). However, the factor  $(\delta \lambda_z)^2$  only expresses the fact that the amplitudes of the leading irrelevant operators vanish *on* the EK line, so that the characteristic logarithmic features appear only in second order in  $\delta \lambda_z$ . The fact that the scale above which these logarithmic features vanish is  $T \simeq \Gamma$ , not  $T \simeq \Gamma/(\delta \lambda_z)^2$ , supports our above conclusion that it is rather  $\Gamma$  that should be identified as the Kondo scale.

### VII. SINGLE-CHANNEL KONDO MODEL

The methods used above can also be applied, with minor modifications, to the single-channel Kondo (1CK) model. This is done in Appendix D. The main difference to the 2CK case is of course that both the weak and strong-coupling fixed points are Fermi liquids, but they are again connected by a line, called the 'Toulouse point,' along which the model is exactly solvable. The main results of Appendix D are summarized in Fig. 4, which shows the finite-size cross-over spectrum of the 1CK model. It nicely illustrates the fact, first discussed by Wilson,<sup>50</sup> that both the two weak- and strong-coupling fixed-point spectra correspond to free fermions, which satisfy, however, different boundary conditions (antiperiodic or periodic, respectively).

## VIII. DISCUSSION AND CONCLUSIONS

The main general conclusion of our work is that constructive finite-size bosonization is an unexpectedly powerful tool for investigating quantum impurity problems. First, for the 2CK model, it enables one to analytically calculate by elementary means the crossover along the EK line of the finitesize spectrum (and the corresponding eigenstates) between the free Fermi liquid and the NFL fixed point. Although the fixed point spectrum had already been obtained by means of conformal field theory,<sup>23,26</sup> this crossover had hitherto been tractable only with the NRG, and has been beyond the reach of all analytical approaches used to study this model. Moreover, the ability to treat the crossover explicitly allowed us to prove in a direct way the two central assumptions on which Affleck and Ludwig's very elegant CFT solution is based, namely, that spin anisotropy is irrelevant so that the NFL fixed point has the same  $U(1)_c \times SU(2)_s \times SU(2)_f$  symmetry as the free model, and the fusion hypothesis for the operator content of the NFL fixed point.

Secondly, finite-size bosonization *can deal without much additional effort with symmetry-breaking perturbations*, such as a finite magnetic field (or channel symmetry breaking,<sup>13</sup> which was not discussed here, but can be included by a straightforward extension of our methods). Indeed, it is to be expected that the methods developed here can fruitfully be applied to a number of related quantum impurity problems. For example, an adaption of our finite-size refermionization approach was very recently used to rigorously resolve a recent controversy regarding the tunneling density of states at the site of an impurity in a Luttinger liquid.<sup>31</sup> Other potential applications would be to the generalized Kondo models studied by Ye,<sup>27</sup> or by Moustakas and Fisher,<sup>25,53</sup> or by Kotliar and Si.<sup>28</sup>

Thirdly, finite-size bosonization allows one *to mimic in an exact way the strategy of standard RG approaches* such as poor man's bandwidth rescaling and finite-size scaling; thus it should be useful also as a pedagogical tool for teaching and analytically illustrating RG ideas.

Coleman and co-workers<sup>12,13</sup> have proposed a "pedestrian solution" of the 2CK model, in which it is argued that many of its properties can be calculated using a so-called "compactified model" involving only a single channel of spinful conduction electrons. This model was argued to represent that part of the 2CK model that is left over when one "factorizes out" the charge and flavor degrees of freedom. Indeed, using field-theoretic bosonization, Schofield showed that there is a formal correspondence between the compactified model and our  $H_{\perp}$  of Eq. (27) (which involves only  $\varphi_s$ and  $\varphi_x$ ), and that it yields the same results as the 2CK model for the *impurity contribution* to thermodynamical properties. In this sense, the compactified model can be viewed as an effective model for calculating impurity properties. However, as first emphasized by Ye,27 it is not equivalent to the original 2CK model, since Schofield's arguments ignored the

fact that there are gluing conditions such as Eq. (20) between the c, f sectors and the s, x sectors. As long as these are ignored, the compactified model can *not* be used to calculate conduction electron properties, since that requires adding back the contributions from the charge and flavor channels.

Our constructive bosonization approach allowed us to clarify this issue completely: it makes precise in what sense the *c* and *f* sectors can be "factorized out," rigorously yields an appropriate model for the remaining *s* and *x* sectors, emphasizes the gluing conditions between the *c*, *f* and *s*, *x* sectors, and shows how they can be used at the NFL fixed point to combine the contributions from all four sectors to obtain the NFL fixed point spectrum. [An alternative way of doing this explicitly was found by Bradley, Bulla, Hewson, and Zhang,<sup>15</sup> using the equivalence of the compactified model to a certain O(3) symmetric Anderson model.] Maldacena and Ludwig<sup>30</sup> have used CFT to show that

Maldacena and Ludwig<sup>30</sup> have used CFT to show that Affleck and Ludwig's CFT solution can be reformulated in terms of free boson fields  $\varphi_y(x)$  satisfying certain asymptotic boundary conditions. Ye<sup>27</sup> reproduced this result using fieldtheoretic bosonization at the EK line (in the continuum limit) invoking scaling arguments. We have shown in Ref. 4 (and will elaborate this in a future publication<sup>36</sup>) that these results can be reproduced with great ease by simply taking the continuum limit  $L \rightarrow \infty$  of our above finite-size calculation. In fact, this allows us to check explicitly Affleck and Ludwig's results for electronic correlations functions.

In summary, using finite-size bosonization we have calculated analytically and from first principles, but in a conceptually straightforward way, the crossover of the finite-size spectrum of the 2CK model from the free to the NFL fixed point. This enabled us to elucidate the nature of the NFL excitations and to perform a detailed finite-size scaling analysis of the NFL fixed point.

## ACKNOWLEDGMENTS

We are deeply indebted to Michele Fabrizio for his invaluable help in the early stages of this work and his careful reading of the manuscript. We are also grateful to Andreas Ludwig and Abraham Schiller for illuminating discussions and generous help, Gabriel Kotliar and Anirvan Sengupta for useful suggestions, and Volker Meden for a discussion on cutoff-related matters. This research has been supported by Grant No. SFB195 of the Deutsche Forschungsgesellschaft and by the Hungarian Grant Nos. OTKA T026327 and OTKA F030041. G.Z. has been supported by the Magyary Zoltán Foundation.

## APPENDICES

The appendices of this paper may be found in Ref. 37.

- <sup>1</sup>P. Nozières and A. Blandin, J. Phys. (Paris) 41, 193 (1980).
- <sup>2</sup>V. J. Emery and S. Kivelson, Phys. Rev. B 46, 10 812 (1992);
   Phys. Rev. Lett. 71, 3701 (1993).
- <sup>3</sup>D. L. Cox and A. Zawadowski, Adv. Phys. 47, 599 (1998).
- <sup>4</sup>J. von Delft, G. Zaránd, and M. Fabrizio, Phys. Rev. Lett. 81, 196 (1998).
- <sup>5</sup>A. Muramatsu and F. Guinea, Phys. Rev. Lett. **57**, 2337 (1986).
- <sup>6</sup>A. A. Abrikosov and A. A. Migdal, J. Low Temp. Phys. **3**, 519 (1970); M. Fowler and A. Zawadowski, Solid State Commun. **9**, 471 (1971).
- <sup>7</sup>K. Vladár, A. Zawadowski, and G. T. Zimànyi, Phys. Rev. B 37, 2001 (1988); 37, 2015 (1988).

PRB 61

6933

- <sup>8</sup>M. Fabrizio, A. Gogolin, and Ph. Nozières, Phys. Rev. Lett. 74, 4503 (1995); Phys. Rev. B 51, 16088 (1995).
- terms of  $b_{q\alpha i}^{\dagger}$ 's.
- <sup>32</sup>That perturbations about the EK line are irrelevant is shown in Ref. 26, and also in Sec. VI C of this paper.
- <sup>33</sup>F. D. M. Haldane, J. Phys. C 14, 2585 (1981).
- <sup>34</sup>M. Fabrizio and A. Gogolin, Phys. Rev. Lett. 78, 4527 (1997).
- <sup>35</sup>A. Furusaki, Phys. Rev. B 56, 9352 (1997).
- <sup>36</sup>J. von Delft and G. Zaránd (unpublished).
- <sup>37</sup>Appendices A–D may be found in the preprint cond-mat/9812182 (by G. Zaránd and J. von Delft), of which the present paper is a somewhat shorter version, or in EPAPS Document No. E-PRBMDO-61-021010, which is a REVTeX version of the present paper, including all Appendices. This document may be retrieved via the EPAPS homepage (http://www.aip.org/ pubservs/epaps.html) or from ftp.aip.org in the directory /epaps/. See the EPAPS homepage for more information
- <sup>38</sup>A. A. Abrikosov, Physics (Long Island City, N.Y.) 2, 5 (1965).
- <sup>39</sup>Y. Shimizu, O. Sakai, and S. Susuki, J. Phys. Soc. Jpn. 67, 2395 (1998); M. Koga and D. Cox, Phys. Rev. Lett. 82, 2575 (1999).
- <sup>40</sup>P. D. Sacramento and P. Schlottmann, Phys. Rev. B 43, 13 294 (1991).
- <sup>41</sup>V. J. Emery and S. A. Kivelson, in Fundamental Problems in Statistical Mechanics VIII, edited by H. van Beijeren and M. H. Ernst (Elsevier, Amsterdam, 1994), pp. 1-24.
- <sup>42</sup>The fusion hypothesis has also been proven by Sengupta and George using bosonization [cond-mat/9702057 (unpublished)], but their proof requires extensive knowledge of CFT, and the assumption that the fixed point is invariant under modular transformations.
- <sup>43</sup>J. Cardy, in Phase Transition and Critical Phenomena II (Academic, New York, 1987), p. 55.
- <sup>44</sup>A. V. Rozhkov, Int. J. Mod. Phys. B **12**, 3457 (1998).
- <sup>45</sup>P. W. Anderson, J. Phys. C 3, 2346 (1970).
- <sup>46</sup>G. Yuval and P. W. Anderson, Phys. Rev. B 1, 1522 (1970); P. W. Anderson, G. Yuval, and D. R. Hamann, ibid. 1, 4464 (1970).
- <sup>47</sup>K. Vladár and A. Zawadowski, Phys. Rev. B 28, 1564 (1983); 28, 1582 (1983); 28, 1596 (1983).
- <sup>48</sup>G. Zaránd and K. Vladár, Phys. Rev. Lett. **76**, 2133 (1996); G. Zaránd, ibid. 77, 3609 (1996).
- <sup>49</sup>J. Gan, N. Andrei, and P. Coleman, Phys. Rev. Lett. 74, 2583 (1993).
- <sup>50</sup>K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
- <sup>51</sup>T. A. Costi, Phys. Rev. Lett. 80, 1038 (1998).
- <sup>52</sup>K. G. Wilson and J. Kogut, Rev. Mod. Phys. 47, 773 (1975).
- <sup>53</sup>C. Dobler, On the Stability of the 2-Channel Kondo Model, Diplomthesis, Universität Karlsruhe, 1998.

- <sup>9</sup>M. H. Hettler, J. Kroha, and S. Hershfield, Phys. Rev. Lett. 73,
- 1967 (1994); Phys. Rev. B 58, 5649 (1998).
- <sup>10</sup>D. L. Cox and A. E. Ruckenstein, Phys. Rev. Lett. 71, 1613 (1993)
- <sup>11</sup>T. S. Kim and D. L. Cox, Phys. Rev. B 55, 12 594 (1997); 54, 6494 (1996); Phys. Rev. Lett. 75, 1622 (1995).
- <sup>12</sup>P. Coleman, L. B. Ioffe, and A. M. Tsvelik, Phys. Rev. B 52, 6611 (1995).
- <sup>13</sup>P. Coleman and A. Schofield, Phys. Rev. Lett. 75, 2184 (1995).
- <sup>14</sup>R. Bulla, A. C. Hewson, and G.-M. Zhang, Phys. Rev. B 56, 11 721 (1997); R. Bulla and A. C. Hewson, Z. Phys. B: Condens. Matter 104, 333 (1997); G.-M. Zhang and A.C. Hewson, Phys. Rev. Lett. 76, 2137 (1996).
- <sup>15</sup>S. C. Bradley, R. Bulla, A. C. Hewson, and G.-M. Zhang, Eur. Phys. J. B 11, 535 (1999).
- <sup>16</sup>D. M. Cragg, P. Lloyd, and P. Nozières, J. Phys. (Paris) 13, 245 (1980).
- <sup>17</sup>H.-B. Pang, Ph.D. dissertation, The Ohio State University, 1992; H.-B. Pang and D. L. Cox, Phys. Rev. B 44, 9454 (1991).
- <sup>18</sup>I. Affleck, A. W. W. Ludwig, H.-B. Pang, and D. L. Cox, Phys. Rev. B 45, 7918 (1992).
- <sup>19</sup>N. Andrei and C. Destri, Phys. Rev. Lett. 52, 364 (1984).
- <sup>20</sup>P. B. Wiegmann and A. M. Tsvelik, Z. Phys. B: Condens. Matter 54, 201 (1985).
- <sup>21</sup>N. Andrei and A. Jerez, Phys. Rev. Lett. 74, 4507 (1995).
- <sup>22</sup>I. Affleck, Nucl. Phys. B **336**, 517 (1990).
- <sup>23</sup>I. Affleck and A. W. W. Ludwig, (a) Nucl. Phys. B 352, 849 (1991); (b) 360, 641 (1991); (c) Phys. Rev. Lett. 67, 3160 (1991); (d) Phys. Rev. B 48, 7297 (1993); (e) Nucl. Phys. B 428, 545 (1994).
- <sup>24</sup>A. W. W. Ludwig, Int. J. Mod. Phys. B 8, 347 (1994).
- <sup>25</sup>A. L. Moustakas and D. S. Fisher, Phys. Rev. B 53, 4300 (1996); 51, 6908 (1995).
- <sup>26</sup>A. M. Sengupta and A. Georges, Phys. Rev. B **49**, 10 020 (1994).
- <sup>27</sup>J. W. Ye, (a) Phys. Rev. Lett. 77, 3224 (1996); (b) 79, 1385 (1997); (c) Nucl. Phys. B 512, 543 (1998).
- <sup>28</sup>G. Kotliar and Q. Si, Phys. Rev. B 53, 12 373 (1996).
- <sup>29</sup>A. Schiller and S. Hershfield, Phys. Rev. B **51**, 12 896 (1995).
- <sup>30</sup>J. M. Maldacena and A. W. W. Ludwig, Nucl. Phys. B 506, 565 (1997).
- <sup>31</sup>Jan von Delft and H. Schoeller, Ann. Phys. (Leipzig) 7, 225 (1998). This review gives an elementary, non-field-theoretic derivation of bosonization, by noting that  $\psi_{\alpha j}(x) | \vec{N} \rangle$  is an eigenstate of  $b_{a\alpha i}$  and hence has a coherent state representation in