

Transition from Overscreening to Underscreening in the Multichannel Kondo Model: Exact Solution at Large N

Olivier Parcollet and Antoine Georges

Laboratoire de Physique Théorique de l'École Normale Supérieure,* 24 rue Lhomond, 75231 Paris Cedex 05, France
(Received 31 July 1997)

A novel large- N limit of the multichannel Kondo model is introduced, for representations of the impurity spin described by Schwinger bosons. Three cases are found, associated with *underscreening*, *overscreening*, and *exact Kondo screening* of the impurity. The saddle-point equations derived in this limit are reminiscent of the “noncrossing approximation,” but preserve the Fermi-liquid nature of the model in the exactly screened case. Several physical quantities are computed, both numerically and analytically in the low- ω, T limit, and compared to other approaches. [S0031-9007(97)04661-9]

PACS numbers: 75.20.Hr, 71.10.Hf, 75.30.Mb

Besides their experimental relevance to magnetic impurities in metals, heavy fermion compounds, and tunneling in mesoscopic systems [1], quantum impurity models provide useful testing grounds for theoretical methods dealing with correlated electron systems. Among those, explicit solutions in the limit of large spin degeneracy [e.g., $SU(N)$ spins in the large N limit] have often proven to retain many crucial aspects of the low-energy physics while being simple to implement [2].

In this Letter, we introduce a novel large- N approach to the multichannel Kondo model [3,4]. The non-Fermi liquid properties of this model in the overscreened regime have attracted considerable attention recently. Our approach is related to the earlier work of Cox and Ruckenstein [5], in that we also consider the $SU(N)$ Kondo model with K channels of conduction electrons and take the limit $N, K \rightarrow \infty$ with $K/N = \gamma$ being fixed. There are two crucial differences with Ref. [5], however: (i) we are dealing here with *Schwinger boson* representations of the impurity spin, in contrast with the fermionic representations considered in [5], and (ii) we keep track of the quantum number associated with the “size” of the impurity spin by imposing a local constraint on the Schwinger bosons which is also taken to scale as N . Because of these two new features, our approach captures all three possible regimes of the multichannel Kondo model (and transitions between them): the *underscreened* regime (in which the Kondo effect only partially screens the impurity spin), the *overscreened* regime (in which a non-Fermi liquid state is formed at low energy), and an *exactly screened* Fermi-liquid regime in between.

In the large- N limit, our model is solved by a set of two coupled integral equations. These equations resemble in structure the “noncrossing approximation” (NCA) [5,6], with some crucial differences, however, associated with points (i) and (ii) above. Because of our handling (ii) of the constraint, these equations result from a true saddle-point principle, with controllable fluctuations in $1/N$. Furthermore, in the exactly screened case, the equations derived in this paper *preserve the local Fermi-liquid*

character of the problem down to zero temperature and frequency. For this reason, and because Schwinger boson mean-field theories yield a quite satisfactory description of magnetically ordered phases [7], our approach offers new prospects for a successful treatment of the Kondo lattice model.

We consider a generalized Kondo model with K channels of conduction electrons and a spin symmetry group extended from $SU(2)$ to $SU(N)$. An impurity spin \vec{S} is placed at the origin. We choose to represent the $N^2 - 1$ components $(S_{\alpha\beta})_{1 \leq \alpha, \beta \leq N}$ of \vec{S} in terms of N Schwinger bosons b_α with a constraint, namely,

$$S_{\alpha\beta} = b_\alpha^\dagger b_\beta - \frac{P}{N} \delta_{\alpha\beta}, \quad \sum_{\alpha=1}^N b_\alpha^\dagger b_\alpha = P. \quad (1)$$

In all the following, the conduction electrons transform under the fundamental representation of $SU(N)$. The Hamiltonian of the model reads

$$H = \sum_{\vec{p}} \sum_{\substack{1 \leq i \leq K \\ 1 \leq \alpha \leq N}} \epsilon_{\vec{p}} c_{\vec{p}i\alpha}^\dagger c_{\vec{p}i\alpha} + J_K \sum_{\vec{p}} S_{\alpha\beta} c_{\vec{p}i\beta}^\dagger c_{\vec{p}'i\alpha}. \quad (2)$$

In the usual $N = 2$ case ($\alpha, \beta = \uparrow, \downarrow$), this is the multichannel Kondo model with an impurity spin of size $S = P/2$. For arbitrary N , Eq. (1) means that we have restricted ourselves to representations of $SU(N)$ corresponding to a Young tableau with a single line of P boxes. Quantum fluctuations are stronger at small values of P , while large P (for fixed N) corresponds to a semiclassical limit.

It is easily checked that a weak antiferromagnetic coupling ($J_K > 0$) grows under renormalization for all K and N , and all representations P of the local spin. In order to determine whether the renormalization group (RG) flow takes J_K all the way to strong coupling (underscreened or exactly screened cases), or whether an intermediate non-Fermi liquid fixed point exists (overscreened case), we have generalized the Nozières and Blandin stability analysis of the strong-coupling fixed point $J_K = +\infty$ [3]. In this limit, a bound state is formed between

the impurity spin and the conduction electrons, which corresponds to a new spin representation dictated by the minimization of the Kondo energy [second term in (2)]. One must then study the stability of this strong-coupling state when a small hopping t of the conduction electrons is turned on. The technical steps involved in this analysis will be reported elsewhere [8,9], and only the main conclusions are summarized here. We have established that, for arbitrary value of N , there are three possible strong-coupling regimes [10] depending on the number of channels K as compared to P :

(i) When $P > K$, $(N - 1)K$ conduction electrons bind to the impurity spin in such a way that a free local spin of size $P^{sc} = P - K$ is left unscreened for $J_K/t = \infty$. Turning on a hopping tends to increase the total spin of the system, corresponding to a weak *ferromagnetic* residual Kondo interaction as one departs from the strong-coupling fixed point. Hence, the latter is stable against this perturbation, and we have the typical situation of an *underscreened* (US) Kondo effect.

(ii) When $P = K$, $(N - 1)K$ conduction electrons exactly screen the impurity spin and produce a spin singlet state ($P^{sc} = 0$). The strong-coupling state, having the lowest possible degeneracy, must again be stable against t/J_K , and the model displays exact Kondo screening (ES).

(iii) When $P < K$, $(N - 1)P$ conduction electrons screen the impurity spin, while $(N - 1)(K - P)$ arrange themselves such that a residual spin $P^{sc} = K - P$ remains. In contrast to the above case, the residual Kondo

interaction produced when a hopping is turned on is now *antiferromagnetic*, and the strong-coupling fixed point is unstable. One expects, as confirmed below, that an intermediate fixed point exists with non-Fermi liquid properties: this is the *overscreened* (OS) regime.

We now turn to the analysis of this model in the large- N limit. We shall proceed in a manner similar to Ref. [5], by setting $K = \gamma N$ and $J_K = J/N$ and taking the limit $N \rightarrow \infty$ for fixed values of γ and J . The crucial difference (apart from the use of Schwinger bosons) is that we shall deal with the constraint in Eq. (1) by setting $P = p_0 N$ and keeping p_0 fixed (instead of fixing $P = 1$ as in [5]). By doing so, we are preserving the existence of the transition in the large- N limit, the three regimes above corresponding to $p_0 > \gamma$ (US), $p_0 = \gamma$ (ES), and $p_0 < \gamma$ (OS). This also ensures that the model is controlled by a *true saddle point* at large N , with controllable $1/N$ corrections.

In order to derive the saddle-point equations, we use a functional integral formulation of model (2), with a Lagrange multiplier field $\lambda(\tau)$ to implement the constraint. Conduction electrons can be integrated out in the bulk, keeping only degrees of freedom at the impurity site. The local Kondo interaction is decoupled by introducing an auxiliary field in each channel $F_i(\tau)$, conjugate to the amplitude $\sum_{\alpha} c_{i\alpha}^{\dagger}(\tau)b_{\alpha}(\tau)$. This field will be responsible for capturing the physics of the Kondo effect. Note that it is a *Grassmannian (anticommuting) field*, because of our bosonic treatment of the impurity spin. After these manipulations, we are left with the effective action,

$$S = \int_0^{\beta} d\tau \sum_{\alpha=1}^N b_{\alpha}^{\dagger}(\tau) \partial_{\tau} b_{\alpha}(\tau) + \frac{1}{J} \int_0^{\beta} d\tau \sum_{i=1}^K F_i^{\dagger} F_i + \frac{1}{N} \int_0^{\beta} \int_0^{\beta} d\tau d\tau' \sum_{i\alpha} F_i(\tau) b_{\alpha}^{\dagger}(\tau) G_0(\tau - \tau') F_i^{\dagger}(\tau') b_{\alpha}(\tau') + \int_0^{\beta} d\tau i\lambda(\tau) \left(\sum_{\alpha} b_{\alpha}^{\dagger}(\tau) b_{\alpha}(\tau) - p_0 N \right). \quad (3)$$

In this expression, $G_0(i\omega_n) \equiv \sum_{\bar{p}} 1/(i\omega_n - \epsilon_{\bar{p}})$ is the on-site Green's function associated with the conduction electron bath. The quartic term in Eq. (3) can be decoupled formally using two bilocal fields $Q(\tau, \tau')$ and $\bar{Q}(\tau, \tau')$ conjugate to $\sum_{\alpha} b_{\alpha}^{\dagger}(\tau)b_{\alpha}(\tau')$ and $\sum_i F_i^{\dagger}(\tau)F_i(\tau')$, respectively. Integrating out all other fields, the action can be solved by a saddle-point method over Q , \bar{Q} , and λ for $N \rightarrow \infty$, which leads to coupled equations for the Schwinger boson and auxiliary field Green's functions $G_b(\tau) \equiv -\langle T b(\tau) b^{\dagger}(0) \rangle$, $G_F(\tau) \equiv -\langle T F(\tau) F^{\dagger}(0) \rangle$ and for the Lagrange multiplier field (the latter is static and purely imaginary at the saddle point: $i\lambda \equiv \bar{\lambda}$). These coupled equations read

$$\Sigma_b(\tau) = \gamma G_0(\tau) G_F(\tau), \quad \Sigma_F(\tau) = G_0(\tau) G_b(\tau), \quad (4)$$

where the self-energies Σ_b and Σ_F are defined by

$$G_b^{-1}(i\nu_n) = i\nu_n + \bar{\lambda} - \Sigma_b(i\nu_n), \\ G_F^{-1}(i\omega_n) = \frac{1}{J} - \Sigma_F(i\omega_n). \quad (5)$$

In these expressions $\omega_n = (2n + 1)\pi/\beta$ and $\nu_n = 2n\pi/\beta$ denote fermionic and bosonic Matsubara frequencies. Finally, $\bar{\lambda}$ is determined by the constraint

$$G_b(\tau = 0^-) \equiv \sum_n G_b(i\nu_n) e^{i\nu_n 0^+} = -p_0. \quad (6)$$

We have studied these equations both numerically and analytically in the limit of low temperature and low energy. The three Kondo regimes are best illustrated by Fig. 1, which displays the zero-temperature limit of the Curie constant $\kappa = \lim_{T \rightarrow 0} T \chi_{\text{imp}}(T)$ and of the impurity entropy $S_{\text{imp}} = \lim_{T \rightarrow 0} \lim_{V \rightarrow \infty} [S(T) - S_{\text{bulk}}(T)]$, as a function of the "size of the spin" p_0 . κ vanishes in the (OS) and (ES) regimes ($p_0 \leq \gamma$), but reaches a finite value $\kappa = (p_0 - \gamma)(p_0 - \gamma + 1)$ in the (US) regime ($p_0 > \gamma$), corresponding to the Curie constant of a residual spin of size $P_{sc} = P - K = N(p_0 - \gamma)$ in the large- N limit. Accordingly, the correlation function of the impurity spin does not vanish at long times in the (US) regime: $\langle S(0)S(\tau) \rangle \sim \text{const}$, while $\langle S(0)S(\tau) \rangle \sim$

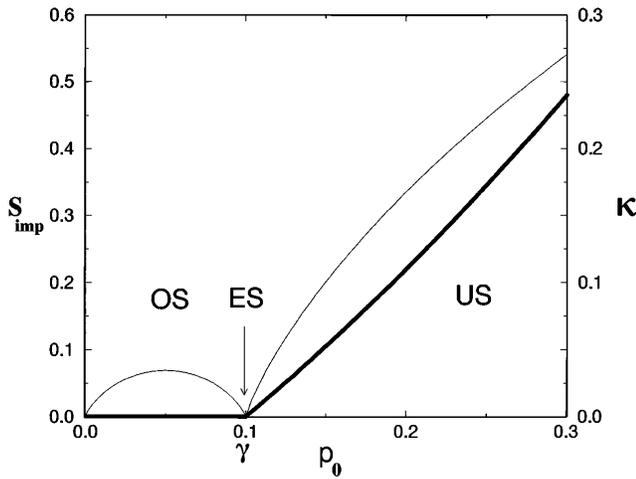


FIG. 1. Residual entropy (thin line) and Curie constant (bold line) vs the “size” of the spin p_0 , for $\gamma = 0.1$ (analytical expressions given in the text).

$1/\tau^{2/(1+\gamma)}$ in the (OS) regime. The latter is the behavior expected from the conformal field theory (CFT) [11] and Bethe ansatz analysis [12] of the non-Fermi liquid (OS) fixed point. The residual entropy at $T = 0$ also takes the value expected from the degeneracy associated with a free spin of size $N(p_0 - \gamma)$ in the (US) regime, namely, $S_{\text{imp}}/N = (p_0 - \gamma + 1) \ln(p_0 - \gamma + 1) - (p_0 - \gamma) \ln(p_0 - \gamma)$, and vanishes at the (ES) point. In the (OS) regime, its value is a universal function of p_0 and γ associated with the non-Fermi liquid fixed point, which will be calculated explicitly below [Eq. (9)].

The crossover between the high-temperature and low-temperature regimes, associated with the Kondo effect, is illustrated in Fig. 2 which displays the “local Curie constant” $T\chi_{\text{loc}}(T)$ vs $\ln T$ in the (US) and (ES) regimes (with $\chi_{\text{loc}} = \int_0^\beta \langle S(0)S(\tau) \rangle d\tau$).

We now turn to a more detailed analysis of the low-energy, low-temperature behavior of the above equations

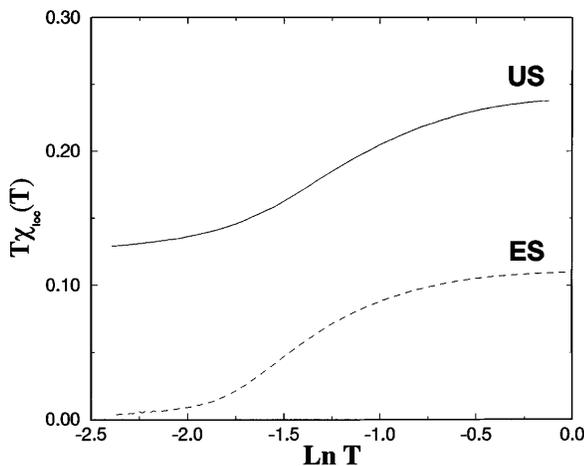


FIG. 2. Numerically calculated local Curie constant $T\chi_{\text{loc}}(T)$ vs $\ln T$ with $\gamma = 0.1$, for $p_0 = 0.1$ (ES case) and $p_0 = 0.2$ (US case).

in the three regimes. In the (OS) case $\gamma > p_0$, we first consider the zero-temperature limit, and perform a long-time asymptotic analysis similar to that made in Ref. [13]. The crucial point in this regime is that the constant terms in the right-hand side of Eq. (5) vanish as $T \rightarrow 0$, namely, $\bar{\lambda} - \Sigma_b(i0^+) \rightarrow 0$, $1/J - \Sigma_F(i0^+) \rightarrow 0$. As a result, a power-law decay $G_b(\tau) \sim A_b/\tau^{2\Delta_b}$, $G_F(\tau) \sim A_F/\tau^{2\Delta_F}$ is found for the Green’s functions in the limit $T_k^{-1} \ll \tau \ll \beta \rightarrow \infty$ (where T_k is the Kondo temperature). The exponents are given by $2\Delta_b = 1/(1 + \gamma)$, $2\Delta_F = \gamma/(1 + \gamma)$, so that the local spin-spin correlation decays as $\langle S(0)S(\tau) \rangle \propto G_b(\tau)G_b(-\tau) \sim 1/\tau^{2/(1+\gamma)}$. The spectral density of the Schwinger boson has the following low-frequency behavior at zero temperature (with C a positive constant):

$$\rho_b(\omega \rightarrow 0^\pm) \sim C \frac{\sin \theta_\pm}{(\pm\omega)^{1-2\Delta_b}}. \quad (7)$$

It is important to observe that the same power-law behavior is found for $\omega > 0$ and $\omega < 0$, but with *asymmetric prefactors* parametrized by the phases θ_\pm . The values of these phases can be found using a Luttinger-Ward argument [8,9], leading to $\sin \theta_+ = \sin \frac{\pi}{1+\gamma}(\gamma - p_0)$, $\sin \theta_- = -\sin \frac{\pi}{1+\gamma}p_0$. From these expressions, we see that Eq. (7) obeys the positivity property appropriate for a bosonic spectral density: $\text{sgn}(\omega)\rho_b(\omega) > 0$ only as long as $p_0 < \gamma$ ($P < K$). The violation of this property signals the transition to the (US) regime, in which the solutions just described are no longer valid.

Contact can be made, at least qualitatively, with the usual NCA equations (enforcing $P = 1$ strictly), and with Ref. [5], by taking the limit $p_0 \rightarrow 0$, i.e., dealing with an impurity such that $P \ll N$. In that case, we observe that $\theta_- \rightarrow 0$, and the $T = 0$ spectral density vanishes for negative frequencies. There is no such threshold for nonzero values of p_0 , however, but the spectral density does become increasingly asymmetric as p_0 gets smaller.

In order to calculate the low-temperature behavior of thermodynamic quantities, the above $T = 0$ form of the spectral densities is insufficient, however. The limit $\omega, T \rightarrow 0$ must be taken while keeping $\tilde{\omega} \equiv \omega/T$ finite [14]. We have succeeded [8,9] in calculating analytically the spectral functions in this limit, which takes a *scaling form*: $\rho_{b,F}(\omega) = A_{b,F}T^{2\Delta_{b,F}-1}\phi_{b,F}(\tilde{\omega})$. The scaling function ϕ_b (found from either a direct solution of the integral equations above, or from conformal field theory arguments) reads

$$\phi_b(\tilde{\omega}; p_0) = \frac{(2\pi)^{2\Delta_b}}{2\pi^2} \sinh \frac{\tilde{\omega}}{2} \frac{|\Gamma(\Delta_b + i\frac{\tilde{\omega} - \tilde{\omega}_0}{2\pi})|^2}{\Gamma(2\Delta_b)}, \quad (8)$$

in which $\tilde{\omega}_0 \equiv \ln|\sin \theta_+/\sin \theta_-|$. ϕ_F has a similar expression, with Δ_F replacing Δ_b and $\cosh \tilde{\omega}/2$ replacing $\sinh \tilde{\omega}/2$. Using Eq. (8) and the expression of the free energy $F_{\text{imp}}/N = -p_0\bar{\lambda} - T \sum_n \ln G_b(i\nu_n) + \gamma T \sum_n \ln G_F(i\omega_n) - T \sum_n \sum_b(i\nu_n)G_b(i\nu_n)$ we have obtained [8,9] the zero-temperature limit of the entropy,

which is a universal number associated with the non-Fermi liquid fixed point [15]. We find

$$\frac{1}{N} S_{\text{imp}} = \frac{1 + \gamma}{\pi} [f_{\gamma}(1 + p_0) - f_{\gamma}(1) - f_{\gamma}(p_0)], \quad (9)$$

with $f_{\gamma}(x) \equiv \int_0^{\pi x/1+\gamma} \ln \sin(u) du$. We have also calculated [8,9] S_{imp} for arbitrary finite values of N, K , and P by applying the CFT methods of Refs. [11,15]. We find (for $K > P$) $S_{\text{imp}} = \ln \prod_{n=1}^P \sin \frac{\pi(N+n-1)}{N+K} / \sin \frac{\pi n}{N+K}$, which can also be established using Bethe ansatz methods [12]. The large- N limit of this expression coincides with (9), with corrections of order $1/N$ [16]. We have also computed the low-temperature behavior of the specific heat ratio and impurity susceptibility in the overscreened regime, and found $C/T \sim \chi_{\text{imp}} \sim 1/T^{(\gamma-1)/(\gamma+1)}$ for $\gamma > 1$, $C/T \sim \chi_{\text{imp}} \sim \ln 1/T$ for $\gamma = 1$, $C/T \sim \chi_{\text{imp}} \sim \text{const}$ for $\gamma < 1$, also in agreement with the CFT and Bethe ansatz results. Note that the last behavior holds even though the fixed point is *not* a Fermi liquid (as evidenced by the fact that $S_{\text{imp}} \neq 0$).

In the (US) regime, the crucial difference with the above analysis is that $1/J - \Sigma_F(i0^+)$ no longer vanishes at zero temperature, but instead *diverges logarithmically*: $1/J - \Sigma_F(i0^+) \sim 1/J_e \ln T + J_2$ [while $\bar{\lambda} - \Sigma_b(i0^+) \sim \lambda_1 T$]. This behavior is well obeyed by the numerical solution of the above equations, and has a simple physical interpretation: in the (US) case, the residual spin is asymptotically free at low temperature, but is weakly coupled to the conduction electron gas at any finite temperature by a *ferromagnetic* Kondo coupling which vanishes logarithmically as temperature is reduced. Based on this observation, we can find the low-temperature scaling form of the spectral functions as $\rho_b(\omega) = \delta(\omega/Z + \lambda_1 T) + \dots$ and $\rho_F(\omega) = 1/\ln^2 T \phi_F(\omega/T) + \dots$. The form of ρ_b is characteristic of an (asymptotically) free local spin. The detailed expression of ϕ_F will be given elsewhere [9].

Finally, we briefly comment on the (ES) case. The large- N limit preserves the local impurity properties expected from the full Kondo screening, namely, $S_{\text{imp}} \rightarrow 0$ and $\chi_{\text{loc}} \rightarrow \text{const}$ as $T \rightarrow 0$. The conduction electrons form a local Fermi liquid which is, however, only weakly affected by the screening of the impurity in the large- N limit. Indeed, the scattering phase shift obtained from Friedel's sum rule is $\delta/\pi = 1/N$. Accordingly, the scattering T matrix, obtained in our approach as the Fourier transform of $G_b(\tau)G_F(-\tau)$, is found to have vanishing imaginary part in the limit of $\omega, T \rightarrow 0$. This is a peculiarity of the specific spin representation that we have considered: considering rectangular Young tableaux with $P = K = \gamma N$ columns and $N/2$ lines would restore maximal unitary scattering $\delta = \pi/2$ for all N . Whether

a large- N limit exists for that case also is an interesting open problem, with potentially useful applications, e.g., to the Kondo lattice model.

During the course of this study, we learned of simultaneous work by N. Andrei, A. Jerez, and G. Zaránd on the same model using the Bethe ansatz method [12]. Our results and conclusions agree when a comparison is possible. We are most grateful to N. Andrei for numerous discussions. We also thank T. Giamarchi, P. Coleman, G. Kotliar, A. Sengupta, A. Ruckenstein, and P. Zinn-Justin for very helpful suggestions.

*Unité propre du CNRS (UP 701) associée à l'ENS et à l'Université Paris-Sud.

- [1] See, e.g., *Correlated Fermions and Transport in Mesoscopic Systems*, edited by T. Martin, G. Montambaux, and J. Tran Thanh Van (Editions Frontieres, Gif-sur-Yvette, France, 1996).
- [2] For reviews, see, e.g., D.M. Newns and N. Read, *Adv. Phys.* **36**, 799 (1987) and G. Kotliar, in *Strongly Interacting Fermions and High T_c Superconductivity*, edited by B. Doucot and J. Zinn-Justin (Elsevier Science Pub., New York, 1994).
- [3] P. Nozières and A. Blandin, *J. Phys. (Paris)* **41**, 193 (1980).
- [4] For a recent review on non-Fermi liquid fixed points in Kondo models, see D.L. Cox and A. Zawadowski, e-print cond-mat/9704103 [Adv. Phys. (to be published)].
- [5] D.L. Cox and A. E. Ruckenstein, *Phys. Rev. Lett.* **71**, 1613 (1993).
- [6] For a review, see N.E. Bickers, *Rev. Mod. Phys.* **59**, 845 (1987).
- [7] A. Auerbach and D.P. Arovas, *Phys. Rev. Lett.* **61**, 617 (1988).
- [8] O. Parcollet, A. Georges, G. Kotliar, and A. Sengupta (to be published).
- [9] O. Parcollet and A. Georges (to be published).
- [10] In all three regimes, the strong-coupling fixed point involves $(N-1)K$ conduction electrons, which combine into an $SU(N)$ representation corresponding to a Young tableau with $N-1$ lines and K columns.
- [11] I. Affleck and A.W.W. Ludwig, *Nucl. Phys.* **B352**, 849 (1991); *Nucl. Phys.* **B360**, 641 (1991).
- [12] N. Andrei (private communication); A. Jerez, N. Andrei, and G. Zaránd (to be published).
- [13] E. Müller-Hartmann, *Z. Phys. B* **57**, 281 (1984); Y. Kuramoto and H. Kojima, *Z. Phys. B* **57**, 95 (1984).
- [14] See also the recent work by S. Sachdev, e-print cond-mat/9705206; e-print cond-mat/9705266.
- [15] I. Affleck and A.W.W. Ludwig, *Phys. Rev. Lett.* **67**, 161 (1991).
- [16] For a numerical calculation of the entropy within the NCA, see T.S. Kim and D.L. Cox, *Phys. Rev. B* **55**, 12594 (1997).