Schwinger Boson Approach to the Fully Screened Kondo Model

J. Rech,[1,2,3] P. Coleman,[1,2] G. Zarand,[1,4] and O. Parcollet[3]

[1]*Kavli Institute for Theoretical Physics, Kohn Hall, University of California at Santa Barbara, Santa Barbara, California 93106, USA*
[2]*Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08855, USA*
[3]*Service de Physique Théorique, CEA/DSM/SPhT-CNRS/SPM/URA 2306, CEA/Saclay, F-91191 Gif-sur-Yvette Cedex, France*
[4]*Theoretical Physics Department, Budapest University of Technology and Economics, Budafoki ut 8. H-1521 Hungary*
(Received 6 July 2005; published 9 January 2006)

We apply the Schwinger boson scheme to the fully screened Kondo model and generalize the method to include antiferromagnetic interactions between ions. Our approach captures the Kondo crossover from local moment behavior to a Fermi liquid with a nontrivial Wilson ratio. When applied to the two-impurity model, the mean-field theory describes the "Varma-Jones" quantum phase transition between a valence bond state and a heavy Fermi liquid.

DOI: 10.1103/PhysRevLett.96.016601 PACS numbers: 72.15.Qm, 71.27.+a, 73.43.Nq, 75.20.Hr

Heavy fermion metals have attracted great interest as an arena for the controlled study of magnetic quantum phase transitions [1]. Several recent observations cannot be understood in terms of the established Moriya-Hertz theory of quantum phase transitions [2–4], including the divergence of the heavy electron masses [5], the near linearity of the resistivity [6–9], and E/T scaling in inelastic neutron spectra [10]. The origins of this failure are thought to be linked to the competition between antiferromagnetism and the screening of local moments via the Kondo effect. It remains an unsolved challenge to discover the appropriate mean-field description and the corresponding quantum critical modes which govern these novel quantum phase transitions [1,11–13].

Large-N methods offer a promising route towards this goal. Historically, these methods played a major role in the theory of classical criticality [14], and more recently, in the theory of heavy fermion metals [15,16]. However, progress on quantum phase transitions has been hindered by our inability to capture both the Kondo effect and antiferromagnetism in the leading large N approximation.

In this Letter, we describe new progress towards this goal using Schwinger's boson representation of spins [17]. Unlike traditional fermionic representations of spin [15,16] the Schwinger boson scheme provides a good description of local moment magnetism [17]. However, efforts to generalize this method to the Kondo problem [18,19] have failed to capture the Fermi liquid physics associated with perfect screening of the moment. Here we solve this problem using a method coinvented by one of us (O. P.) [18] which employs a multichannel Kondo model with K screening channels. By tuning the size of the spin S from $S < K/2$ to $S > K/2$, one can describe both the overscreened and underscreened Kondo models. Difficulties were encountered in past work that appeared to exclude treatment of the perfectly screened case, $2S = K$. We show how these difficulties are overcome to reveal the perfectly screened Fermi liquid and we demonstrate how this method captures the competition with antiferromagnetism in its simplest extension to the two-impurity Kondo model.

We begin with the single impurity Kondo model,

$$\begin{aligned} \mathcal{H} &= \sum_{\vec{k},\nu,\alpha} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}\nu\alpha} c_{\vec{k}\nu\alpha} + H_I - \lambda(n_b - 2S), \\ H_I &= \frac{J_K}{N} \sum_{\nu\alpha\beta} \psi^{\dagger}_{\nu\alpha}\psi_{\nu\beta} b^{\dagger}_{\beta} b_{\alpha}. \end{aligned} \tag{1}$$

In this version of the model, $c^{\dagger}_{\vec{k}\nu\alpha}$ creates a conduction electron of momentum $\vec{k}$, channel index $\nu \in [1, K]$, spin index $\alpha \in [-j, j]$, where $N = 2j + 1$ is even. $\psi^{\dagger}_{\nu\alpha} = \frac{1}{\sqrt{\mathcal{N}_s}} \sum_{\vec{k}} c^{\dagger}_{\vec{k}\nu\alpha}$ creates an electron in the Wannier state at the origin, where $\mathcal{N}_s$ is the number of sites in the lattice. The operator $b^{\dagger}_{\alpha}$ creates a Schwinger boson ("spinon") with spin index $\alpha \in [-j, j]$. The local spin operator is represented by $S_{\alpha\beta} = b^{\dagger}_{\alpha} b_{\beta} - \delta_{\alpha\beta}/N$ and the system is restricted to the physical Hilbert space by requiring $n_b \equiv \sum_{\alpha} b^{\dagger}_{\alpha} b_{\alpha} \equiv 2S$. The final term in H contains a temperature-dependent chemical potential $\lambda(T)$ that implements the constraint $\langle n_b \rangle = 2S$. We will examine the fully screened case $2S = K$, taking the limit $N \to \infty$ with $k = K/N$ fixed.

The first step is to factorize the interaction in terms of auxiliary spinless fermion fields ("holons"), χ_{ν},

$$H_I \to \sum_{\nu\alpha} \frac{1}{\sqrt{N}} [(\psi^{\dagger}_{\nu\alpha} b_{\alpha}) \chi^{\dagger}_{\nu} + \text{H.c.}] + \sum_{\nu} \frac{\chi^{\dagger}_{\nu}\chi_{\nu}}{J_K}. \tag{2}$$

Following the steps outlined by us in earlier work [20], we now write the free energy as a Luttinger-Ward [21] functional of the one particle Green's functions,

$$F[\mathcal{G}] = T\mathrm{Str}[\ln(-\mathcal{G}^{-1}) + (\mathcal{G}_0^{-1} - \mathcal{G}^{-1})\mathcal{G}] + Y[\mathcal{G}], \tag{3}$$

where $\mathrm{Str}[A] = \mathrm{Tr}[A_B] - \mathrm{Tr}[A_F]$ is the graded (super) trace over the Matsubara frequencies, internal quantum numbers of the bosonic (B) and fermionic (F) components of A. $\mathcal{G}_0$ is the bare propagator and $\mathcal{G} = \mathrm{Diag}[\underline{G}_b, \underline{G}_{\chi}, \underline{G}_c]$, the fully dressed propagator, where

$$\begin{aligned}\underline{G}_b(i\nu_n) &= [i\nu_n + \lambda - \Sigma_b(i\nu_n)]^{-1}\delta_{\alpha\alpha'},\\ \underline{G}_\chi(i\omega_n) &= [-J_K^{-1} - \Sigma_\chi(i\omega_n)]^{-1}\delta_{\nu\nu'},\\ \underline{G}_c(i\omega_n) &= [G_{c0}^{-1}(i\omega_n) - \Sigma_c(i\omega_n)]^{-1}\delta_{\alpha\alpha'}\delta_{\nu\nu'}.\end{aligned} \tag{4}$$

$\Sigma(i\omega_n) = \mathcal{G}_0^{-1} - \mathcal{G}^{-1}$ denotes the corresponding self-energies. $G_{c0}(i\omega_n) = \sum_{\vec{k}} 1/(i\omega_n - \epsilon_{\vec{k}})$ is the bare conduction electron Green's function. The quantity $Y[\mathcal{G}]$ is the sum of all closed-loop two-particle irreducible skeleton Feynman diagrams. In the large N limit, we take the leading $O(N)$ contribution to Y (Fig. 1).

The variation of Y with respect to $\mathcal{G}$ generates the self-energy $\delta Y/\delta \mathcal{G} = \Sigma$, which yields $\Sigma_c(\tau) = \frac{1}{N} G_\chi(-\tau) \times G_b(\tau)$. Since Σ_c is of order $O(N^{-1})$ we use the bare conduction propagator G_{c0} in the self-consistent equations,

$$\Sigma_\chi(\tau) = G_b(\tau)G_{c0}(-\tau), \qquad \Sigma_b(\tau) = -kG_\chi(\tau)G_{c0}(\tau). \tag{5}$$

In practice, we solve these equations using a real time representation of the Green's functions. [See, for example, [19]].

The original work in [18,22] focused primarily on the overscreened Kondo model, where $K > 2S$. The perfectly screened case presented two difficulties. First, the requirement that $K = 2S$ appeared extremely stringent, the slightest deviation from this condition leading to singular departures from Fermi liquid behavior at low temperatures. Second, the conduction electron phase shift δ_c is π/N, suggesting that the effect of the Kondo resonance would completely vanish in the large N limit.

Two new observations shed new light on this problem. First, the perfectly screened case is a stable "filled shell" singlet configuration of the spins, which at strong coupling correspond to "rectangular" Young tableau representations of $SU(N)$. [23,24]. In our gauge theory description of the Kondo model, this stability manifests itself through the formation of a gap in the spinon and holon spectrum. When the chemical potential, λ, lies within this gap, the ground-state Schwinger boson occupancy locks into the value $n_b = K = 2S$ (Fig. 2). Moreover, the gap removes the effect of the spinons and holons at low energies to reveal a Fermi liquid.

Second, although the conduction phase shift δ_c is π/N, its effect on the thermodynamics is multiplied by the N spin components and the K scattering channels, producing an order $O(N \times K/N) \equiv O(N)$ contribution to the free energy. Moreover, a Ward identity $\delta_c = \delta_\chi/N$, where $\delta_\chi = \mathrm{Im}\ \ln[1 + J_K\Sigma_\chi(0 - i\delta)]$ is the (finite) holon phase shift [19,20] enables us to compute the conduction electron scattering in the large N limit.

In the large N limit the entropy [20] is given by

$$\begin{aligned}\frac{S(T)}{N} = \int \frac{d\omega}{\pi}\Big\{ &\frac{dn_B(\omega)}{dT}[\mathrm{Im}\ \ln(-G_b^{-1}) + G_b'\Sigma_b'']\\ &+ k\frac{dn_F(\omega)}{dT}[\mathrm{Im}\ \ln(-G_\chi^{-1}) + G_\chi'\Sigma_\chi'' - G_{c0}''\tilde{\Sigma}_c']\Big\},\end{aligned} \tag{6}$$

where frequency labels ω are suppressed in the integrand, $n_{B/F}$ denote the Bose-Fermi functions, and

$$\begin{aligned}\tilde{\Sigma}_c(\omega) = N\Sigma_c(\omega) = -\int\frac{d\nu}{\pi}\Big\{&\Big[\frac{1}{2} - n_F(\nu)\Big]G_\chi''(\nu)G_b(\omega+\nu)\\ &+\Big[\frac{1}{2} + n_B(\nu)\Big]G_b''(\nu)G_\chi^*(\nu-\omega)\Big\}\end{aligned} \tag{7}$$

is the rescaled conduction self-energy. The shortened notation $G(\omega) = G(\omega - i\delta)$ has been used. We can also calculate the local magnetic susceptibility

$$\chi_{\mathrm{loc}}(T) = -2N\int\frac{d\omega}{\pi}\Big[\frac{1}{2} + n_B(\omega)\Big]G_b'(\omega)G_b''(\omega), \tag{8}$$

where we have taken the magnetic moment of the local impurity to be $M = \sum_\alpha \mathrm{sgn}(\alpha) b_\alpha^\dagger b_\alpha$. Note in passing that the dynamic counterpart $\langle S(t)S(0)\rangle$ vanishes exponentially due to the gap in the bosonic spectral functions, the $1/t^2$ term characteristic of a Fermi liquid only appearing at the next order in $1/N$.

We have numerically solved the self-consistent equations for the self-energy by iteration, imposing the constraint at each temperature. Figure 3 shows the temperature-dependent specific heat coefficient $\frac{C_V}{T} = \frac{dS}{dT}$ and the *full* magnetic susceptibility $\chi(T)$. There is a smooth crossover from local moment behavior at high temperatures $\chi \sim n_b(1 + n_b)/T$ to Fermi liquid behavior at low temperatures. From a Nozières-Blandin description of the local Fermi liquid [25] (where channel and charge suscep-

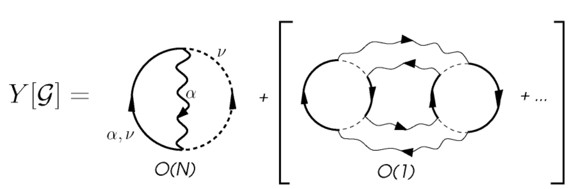

FIG. 1. Leading contributions to $Y[\mathcal{G}]$ in $1/N$ expansion. Solid, dashed, and wavy lines, respectively, represent G_c, G_χ, and G_b. Each vertex is associated with a factor $i/\sqrt{N}$. Bracketed terms are dropped in the large N limit.

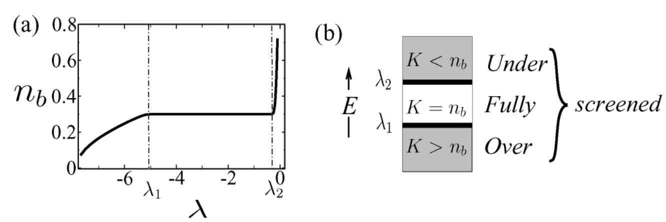

FIG. 2. (a) Calculated variation of occupancy as a functional of boson chemical potential λ in the ground state for $k = 0.3$ and $T/T_K = 0.005$. (b) A spinon gap develops in the fully screened state.

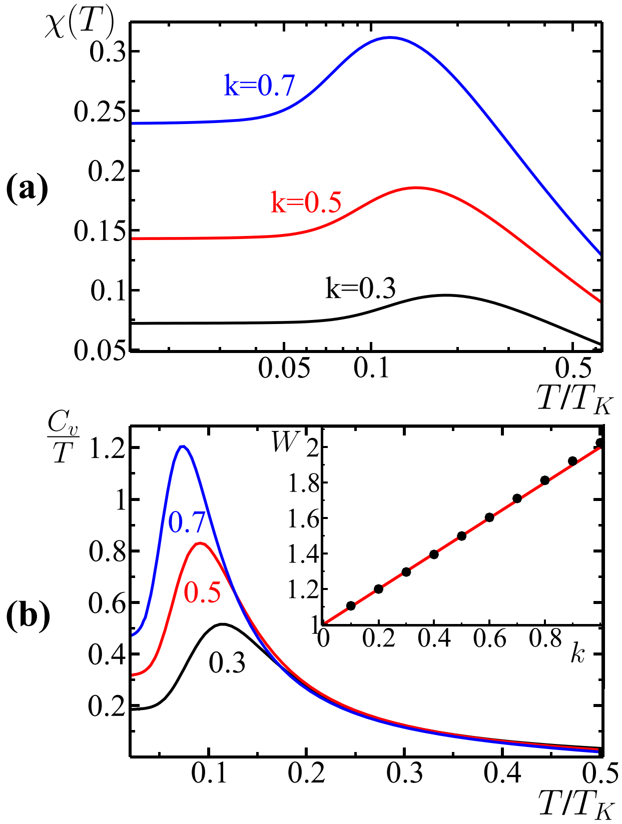

FIG. 3 (color online). Showing temperature dependence of (a) impurity magnetic susceptibility and (b) specific heat capacity in the fully screened Kondo model for $k = 0.3, 0.5, 0.7$ (with the Kondo temperature given by $T_K = De^{-2D/J_K}$, D being the electron bandwidth). Inset calculated Wilson ratio.

tibility vanish), we deduce the Wilson ratio

$$W = \frac{\chi/\gamma}{\chi_0/\gamma_0} = \frac{(1+k)}{1-1/N^2}. \tag{9}$$

This form is consistent with Bethe Ansatz results [23]. We may also derive this result by applying Luttinger-Ward techniques [26] to our model. Our large N approximation reproduces the limiting large N behavior of this expression, $W = 1 + k$; in other words, the local Fermi liquid is interacting in this particular large N limit.

Having demonstrated that our method captures the thermodynamic aspects of the Fermi liquid behavior in the single impurity model, we now show it can handle magnetic correlations within the two-impurity Kondo model,

$$H = \sum_{\vec{k},\nu,\alpha} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}\nu\alpha} c_{\vec{k}\nu\alpha} + H_K(1) + H_K(2) - \frac{J_H}{N} B^{\dagger}_{12} B_{12}, \tag{10}$$

where $H_K(i)$ is the Kondo Hamiltonian for impurity (i) and the antiferromagnetic interaction between the two moments is expressed in terms of the boson pair operator $B_{12} = \sum_\alpha \mathrm{sgn}\,(\alpha) b_{1\alpha} b_{2-\alpha}$. H is invariant under spin transformations in the symmetry group SP (N) (N-even) [27].

We now factorize the antiferromagnetic interaction [17],

$$-\frac{J_H}{N} B^{\dagger}_{12} B_{12} \to \bar{\Delta} B_{12} + B^{\dagger}_{12} \Delta + \frac{N \bar{\Delta} \Delta}{J_H}. \tag{11}$$

Boson pairing is associated with the establishment of short-range antiferromagnetic correlations. Once Δ becomes nonzero, the local gauge symmetry is broken, and the Schwinger bosons propagate from site to site. In this state, the holons delocalize, giving rise to a mobile, charged yet spinless excitation that is gapped in the Fermi liquid. Loosely speaking, on a lattice, these excitations are mobile Kondo singlets. However, since the paired Schwinger bosons interconvert from particle to hole as they move, they only induce holon motion within the *same* sublattice. Therefore, in the special case of two-impurity model, so long as the net coupling between the spins is antiferromagnetic, the holons remain localized.

Under these conditions, we can adapt the single impurity equations to the two-impurity model by replacing

$$G_b(\omega) \to \tilde{G}_b(\omega) = [G_b(\omega)^{-1} - |\Delta|^2 G_b(-\omega)^*]^{-1} \tag{12}$$

in the integral equations. We must also impose self-consistency $\Delta = -J_H \langle B_{12} \rangle$, or

$$\frac{1}{J_H} = -\int \frac{d\omega}{\pi} \mathrm{Im}\left(\frac{1 + 2n_B(\omega)}{G_b^{-1}(\omega) G_b^{-1}(-\omega)^* - |\Delta|^2} \right). \tag{13}$$

We have solved the integral equations with this modified boson propagator. Using the entropy as a guide, we are able to map out the phase diagram (Fig. 4.).

We find that the development of $\Delta \neq 0$ preserves the linear temperature dependence of the entropy at low temperatures, indicating Fermi liquid behavior. However, as the J_H increases, the confining gap for the creation of free spinons and holons collapses towards zero, and the corresponding temperature range of Fermi liquid behavior ultimately vanishes at a critical value of $J_H = J_c$. For $J_H > J_c$, the holon-spinon gap becomes finite again and Fermi liquid behavior reemerges, but the phase shift δ_χ is found to have jumped from π to zero, indicating a collapse of the Kondo resonance. The entropy develops a finite value at the quantum critical point which is numerically identical to half the high temperature entropy of a local moment, $(N/2)[(1 + n_b)\ln(1 + n_b) - n_b \ln n_b]$. Similar behavior occurs at the "Varma-Jones" fixed point [28–30] in the $N = 2$ two-impurity model when the conduction band is particle-hole symmetric. We can in fact identify two maxima in the specific heat, indicating that as in the $N = 2$ Varma-Jones fixed point, the antiferromagnetic coupling generates a second set of screening channels, leading to a two-stage quenching process.

The survival of the Varma-Jones fixed point at large N in the absence of particle-hole symmetry is a consequence of the two-impurity Friedel sum rule,

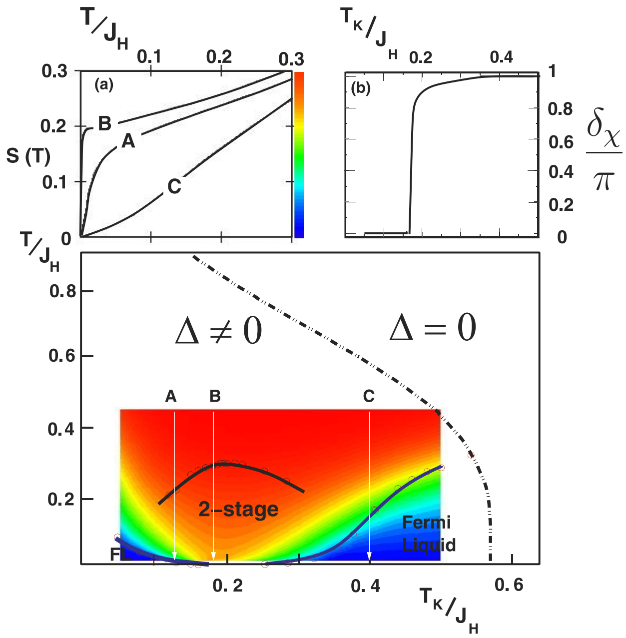

FIG. 4 (color online). Phase diagram for the two-impurity Kondo model showing the boundary where boson pairing develops. Color coded contours delineate the entropy around the Varma-Jones fixed point. Black line indicates upper maximum in specific heat, blue line, lower maximum in specific heat where crossover into the Fermi liquid takes place. Inset: (a) entropy for various values of T_K/J_H, (b) showing dependence of δ_χ on T_K/J_H at a temperature $T/T_K = 0.02$.

$$(\delta_+ + \delta_-) = \frac{2\pi}{N}, \tag{14}$$

where $\delta_\pm$ are the even and odd parity scattering phase shifts. For $N = 2$, it is possible to cross smoothly from unitary scattering off both impurities ($\delta_\pm = \frac{\pi}{2}$), to no scattering off either ($\delta_+ = \pi$, $\delta_- = 0$) while preserving the sum rule, but for $N > 2$, the sum rule cannot be satisfied in the absence of scattering, and the collapse of the Kondo effect must occur via a critical point.

In conclusion, we have shown that a Schwinger boson approach to the fully screened Kondo model can be naturally extended to incorporate magnetic interactions. In the simplest case of a two-impurity Kondo model our approach captures the transition between the state where the two impurities are antiferromagnetically correlated and the Kondo Fermi liquid state. In the large N limit, these two states are separated by a quantum critical point, a possible precursor of an antiferromagnetic quantum critical point. One of the interesting new elements is the appearance of mobile, yet gapped "holon" excitations in the antiferromagnetically correlated Fermi liquid. In the two-impurity model these holons become gapless at the quantum critical point. Future work will examine whether this same scenario also operates at a heavy electron quantum critical point, leading to quantum critical matter with spin-charge decoupling [1,13].

We are grateful to Matthew Fisher, Kevin Ingersent, Andreas Ludwig, and Catherine Pépin for discussions related to this work. This research was supported by the National Science Foundation Grants No. DMR-0312495, No. INT-0130446, and No. PHY99-07949, and the Hungarian National Science Foundation Grant No. OTKA T46303. J.R. and O.P. are supported by an ACI grant of the French Ministry of Research. The authors would like to thank the hospitality of the KITP, where part of this research was carried out.

[1] P. Coleman, C. Pépin, Q. Si, and R. Ramazashvili, J. Phys. Condens. Matter **13**, R723 (2001).
[2] T. Moriya and J. Kawabata, J. Phys. Soc. Jpn. **34**, 639 (1973); **35**, 669 (1973).
[3] J. A. Hertz, Phys. Rev. B **14**, 1165 (1976).
[4] A. J. Millis, Phys. Rev. B **48**, 7183 (1993).
[5] J. Custers *et al.*, Nature (London) **424**, 524 (2003).
[6] H. v. Lohneysen *et al.*, Phys. Rev. Lett. **72**, 3262 (1994).
[7] N. Mathur *et al.*, Nature (London) **394**, 39 (1998).
[8] M. Grosche *et al.*, J. Phys. Condens. Matter **12**, L533 (2000).
[9] O. Trovarelli *et al.*, Phys. Rev. Lett. **85**, 626 (2000).
[10] A. Schroeder *et al.*, Nature (London) **407**, 351 (2000).
[11] Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature (London) **413**, 804 (2001).
[12] T. Senthil, S. Sachdev, and M. Vojta, Physica (Amsterdam) **359-361B**, 9 (2005).
[13] C. Pépin, Phys. Rev. Lett. **94**, 066402 (2005).
[14] K. G. Wilson, Phys. Rev. D **7**, 2911 (1973).
[15] N. Read and D. M. Newns, J. Phys. C **16**, 3273 (1983).
[16] A. Auerbach and K. Levin, Phys. Rev. Lett. **57**, 877 (1986).
[17] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[18] O. Parcollet and A. Georges, Phys. Rev. Lett. **79**, 4665 (1997); O. Parcollet, A. Georges, G. Kotliar, and A. Sengupta, Phys. Rev. B **58**, 3794 (1998).
[19] P. Coleman and I. Paul, Phys. Rev. B **71**, 035111 (2005).
[20] P. Coleman, I. Paul, and J. Rech, Phys. Rev. B **72**, 094430 (2005).
[21] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[22] O. Parcollet, Ph.D. thesis, 1998, http://www-spht.cea.fr/pisp/parcollet/ (unpublished).
[23] A. Jerez, N. Andrei, and G. Zarand, Phys. Rev. B **58**, 3814 (1998).
[24] N. Andrei and P. Zinn Justin, Nucl. Phys. **B528**, 648 (1998).
[25] P. Nozières and A. Blandin, J. Phys. (France) **41**, 193 (1980).
[26] A. Yoshimori, Prog. Theor. Phys. **55**, 67 (1976).
[27] N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991).
[28] B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987).
[29] B. A. Jones, B. G. Kotliar, and A. J. Millis, Phys. Rev. B **39**, 3415 (1989).
[30] J. Gan, Phys. Rev. Lett. **74**, 2583 (1995).