# Kondo cloud and spin-spin correlations around a partially screened magnetic impurity

László Borda,[1] Markus Garst,[2] and Johann Kroha[1]

[1]*Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Nussallee 12, D-53115 Bonn, Germany*
[2]*Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany*

We consider the spatial spin correlations around a partially screened spin-1 magnetic moment in a metal exhibiting the underscreened Kondo effect. We find that the underscreening of the impurity spin results in spatial spin correlations that are more pronounced as compared to the fully screened Kondo effect; their power-law decay is weaker but with characteristic logarithmic corrections at large distances. The spin correlator also changes sign as a function of distance to the impurity allowing for ferromagnetic correlations between conduction-electron spin density and the local moment. The numerical findings are shown to be in agreement with the predictions deriving from an effective ferromagnetic Kondo Hamiltonian.

## I. INTRODUCTION

Spatial spin correlations around Kondo impurities—the Kondo spin screening cloud—and its possible observability in experimental setups have been studied intensively over the last decades.[1–7] Most of the work focused on the properties of spin correlations within the spin-$\frac{1}{2}$ Kondo model, which is thought to capture the essential low-energy physics of magnetic ions in metals. It exhibits complete spin screening and Fermi-liquid behavior below the Kondo temperature $T_K$; two characteristic features that also determine the long-distance behavior of the spin correlations. However, most transition-metal and rare-earth atoms have a spin magnetic moment $S$ greater than $\frac{1}{2}$ in the ground state. Hence, when immersed in a metal they can potentially form underscreened Kondo impurity systems, even if the local-moment degeneracy is partially lifted due to crystal field or spin-orbit splitting.

The ground state of the spin-1 single-channel Kondo model—the prototype of underscreened Kondo models—is known to be effectively a Nozières Fermi liquid with a decoupled impurity spin-$\frac{1}{2}$. Indeed, a careful analysis of the conduction-electron scattering matrix[8,9] revealed that the spectrum exhibits a one-to-one correspondence to that of a free Fermi gas. However, the residual ferromagnetic interaction of the Nozières quasiparticles with the residual impurity spin-$\frac{1}{2}$ (Refs. 10 and 11) results in nonanalytic Fermi-liquid corrections. Although there are well-defined quasiparticles at the Fermi surface, their decay rate vanishes with energy in a singular fashion. Correspondingly, the low-energy properties of the underscreened Kondo models were termed as *singular Fermi-liquid* behavior,[8] in particular, to contrast it with the genuine non-Fermi-liquid characteristics of the overscreened Kondo models. The anomalous corrections should affect all physical quantities that involve the conduction-electron scattering matrix, e.g., conductivity or, as we show below, the long-distance tail of the spin correlations.

Generally, underscreened Kondo physics emerges if the effective number of screening channels that couple to the local moment carrying a spin $S$ is smaller than $2S$. Although the ground state of a Kondo spin in experimental systems is a fully screened singlet in most of the cases, there might be an extended temperature regime with an underscreened mo-

ment as the coupling of some of the channels can be very weak. For example, the screening of a magnetic impurity atom with spin $S > \frac{1}{2}$ adsorbed on metallic surfaces is restricted due to the lower symmetry near the surface potentially giving rise to underscreening.[12,13] A realization in quantum dot setups was also proposed.[14,15] If a quantum dot with a spin $S=1$ ground state is asymmetrically attached to leads, the spin is quenched in a two-stage process. The stronger coupled channel first screens half of the spin-1 at a temperature $T_{K1}$, and the weaker coupled channel subsequently screens the residual spin-$\frac{1}{2}$ at a lower temperature $T_{K2}$. For intermediate temperatures $T_{K2} < T < T_{K1}$, the quantum dot system is governed by the characteristics of the underscreened spin-1 Kondo model and its singular dynamics might be experimentally accessible in this temperature range.

In this work, we focus on the spatial equal-time spin correlations of the conduction electrons around a spin-1 impurity that provide a snapshot of the screening cloud. In general, the characteristics of the screening cloud in Kondo models are less well studied than thermodynamic or transport properties. In the fully screened spin-$\frac{1}{2}$ model, a number of theoretical results[2,3,6] support the expectation that the spatial spin correlations exhibit a crossover at a length scale $\xi_K \equiv \hbar v_F/(k_B T_K)$, where $v_F$ is the Fermi velocity and $T_K$ is the Kondo temperature;[3] for a review, see Sec. 9.6 of Ref. 1. Generally at zero temperature, spin-density correlations decay as a power law with increasing distance $x$ from the impurity. For the fully screened spin-$\frac{1}{2}$ impurity, the crossover is accompanied by a change in the power-law exponent; while at short distances $x < \xi_K$, spin correlations decay as $1/x^d$, with $d$ the dimensionality of the conduction-electron system, there is a stronger $1/x^{d+1}$ decay at large distances $x > \xi_K$.[2,3,6] Recently, it was shown that even the charge-density oscillations around the fully screened impurity bear signatures of this crossover,[7] albeit with much weaker characteristics. On the experimental side, the detection of this crossover in spatial correlations has proved to be elusive so far. The most promising system for its observation is probably a magnetic impurity placed on a metallic surface subject to an scanning tunnel microscope (STM) study.[7]

Comparatively, only little is known about the spatial correlations around a partially screened magnetic impurity. The

question arises as to how the singular Fermi-liquid properties of the underscreened spin-1 Kondo model modify the crossover at $\xi_K$. The scattering of the electrons off the unscreened residual moment will influence the long-distance behavior of spatial correlations, and the conduction-electron cloud around a partially screened impurity—the "underscreening" cloud—will thus differ from its fully screened counterpart. We study this question numerically with the help of an extension of Wilson's numerical renormalization-group (NRG) technique.[6] We find that within the numerical accuracy the envelope of the equal-time impurity-spin electron-spin correlator is a universal function of $x/\xi_K$. In contrast to the spin-$\frac{1}{2}$ model, its power-law decay obtains now only logarithmic corrections for $x > \xi_K$ and its long-distance tail is thus more pronounced than in the fully screened case. We demonstrate that this numerically observed tail of the "underscreening cloud" is in agreement with the predictions of an effective ferromagnetic spin-$\frac{1}{2}$ Kondo model describing the scattering off the residual magnetic moment.

## II. MODEL AND DEFINITION OF CORRELATION FUNCTIONS

The Hamiltonian of the spin-1 single-channel Kondo model reads as

$$\mathcal{H} = J\vec{S}_{\text{imp}}\vec{s}(0) + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}, \tag{1}$$

where $\vec{S}_{\text{imp}}$ is the impurity spin-1 located at $x=0$ and $c_{k\sigma}^{\dagger}$ ($c_{k\sigma}$) creates (annihilates) a conduction electron with momentum $k$ and spin $\sigma$. The impurity spin is antiferromagnetically ($J > 0$) and locally coupled to the electron-spin density $\vec{s}(x) = \psi_{\alpha}^{\dagger}(x)\frac{\vec{\sigma}_{\alpha\beta}}{2}\psi_{\beta}(x)$, with $\psi(x) = \sum_k e^{ikx} c_{k\sigma}$. We limit ourselves here to the case of one-dimensional conduction electrons $d = 1$. A perturbative treatment of the coupling $J$ encounters logarithmic low-energy divergencies that result in a breakdown of perturbation theory at an energy scale $k_B T_K \sim De^{-1/(\nu J)}$, where $D$ is an energy cutoff and $\nu$ is the electron density of states. At energies below $T_K$, the impurity spin gets partially screened from $S_{\text{imp}} = 1$ to $S_{\text{imp}}^* = \frac{1}{2}$ (Ref. [10]) by the conduction electrons which, as a consequence, acquire a phase shift of $\delta_0 = \pi/2$. However, the residual moment $S_{\text{imp}}^*$ still couples ferromagnetically to the electron-spin density.[11] The ferromagnetic spin-$\frac{1}{2}$ Kondo model complemented by an additional phase shift of $\delta_0 = \pi/2$ for the conduction electrons is thus expected to capture the properties of the Hamiltonian (1) at low energies.

Although a ferromagnetic Kondo coupling is marginally irrelevant in the renormalization-group (RG) sense, it results in important corrections to the Fermi-liquid properties. Upon RG improvement, the effective ferromagnetic coupling acquires an energy dependence $\nu J_{\text{eff}}(\varepsilon) = -1/\log(k_B T_K^*/\varepsilon)$ for $\varepsilon \ll k_B T_K^*$ where one identifies $T_K^* \sim T_K$. This logarithmic energy dependence is at the origin of the singular Fermi-liquid properties of the underscreened spin-1 Kondo model. Calculating the phase shift for the conduction electrons in the Born approximation in $J_{\text{eff}}$, one obtains, for example, in a small magnetic field $g\mu_B B \ll k_B T_K$, the spin-dependent correction to $\delta_0 = \pi/2$,

$$\delta_{\sigma} = \frac{\pi}{2}\left(1 + \sigma\frac{1}{2\log(k_B T_K/g\mu_B B)}\right). \tag{2}$$

The focus of the present study is the waves within the Fermi sea that surge around the spin-1 impurity. A snapshot of these is provided by the equal-time correlator of the impurity spin and the conduction-electron spin density at position $x$,

$$\chi(x,T) = \langle \vec{S}_{\text{imp}}\vec{s}(x)\rangle. \tag{3}$$

We also consider the integrated correlator $\chi(T) = \int dx \chi(x,T)$. Using the rotational invariance of the Hamiltonian (1), the latter can be expressed as an expectation value of the $z$ component of the impurity spin $S_{\text{imp}}^z$ and total spin $S_{\text{tot}}^z = S_{\text{imp}}^z + \int dx s^z(x)$,

$$\chi(T) = 3\langle S_{\text{imp}}^z S_{\text{tot}}^z\rangle - 2. \tag{4}$$

This relation is particularly useful for a numerical evaluation of $\chi(T)$ with the help of the NRG.

## III. METHOD

Generally, the calculation of spatial correlations is a nontrivial task since most of the methods used to investigate Kondo models are not able to reproduce correlation functions. One of the most powerful numerical methods, Wilson's NRG, was believed to be unable to handle spatial correlations for a long time. Only very recently it has been extended to have good spatial resolution by one of the authors.[6] The approach is similar to which was used to handle the two impurity problem with NRG.[16] The key idea behind that method is to map the single-channel problem onto an effectively two channel case in order to have good spatial resolution not only around the position of the impurity but around another freely chosen point $x$ as well. For the technical details, we refer the reader to Ref. [6]. In such a scheme, the computation of the equal-time correlation function is rather simple: $\chi(x,T)$ appears to be a static thermodynamic quantity which can be evaluated with a high precision.

## IV. RESULTS

The numerically evaluated correlator $\chi(x,T)$ for different Kondo couplings $J$ (and one-dimensional conduction electrons) is shown in Fig. 1(a). It exhibits characteristic $2k_F$ oscillations, where $k_F$ is the Fermi momentum. Very close to the impurity $xk_F \ll 1$, as well as at distances corresponding to integer multiples of $\pi/k_F$, the spin of the conduction electrons is antiferromagnetically aligned with the impurity spin. In between, $\chi(x,T)$ changes its sign and shows ferromagnetic correlations. Upon excluding the immediate vicinity of the impurity, i.e., distances smaller than $\pi/k_F$, we find that the correlator collapses to a universal curve of the form,

$$\chi(x,T)|_{x>\pi/k_F} = \frac{1}{\xi_K}\left[\mathcal{X}_{2k_F}\left(\frac{x}{\xi_K}, \frac{T}{T_K}\right)\cos(2k_F x + 2\delta_0)\right.$$
$$\left. + \mathcal{X}_{\text{un}}\left(\frac{x}{\xi_K}, \frac{T}{T_K}\right)\right], \tag{5}$$

with two universal functions $\mathcal{X}_{2k_F}$ and $\mathcal{X}_{\text{un}}$. Note that this is
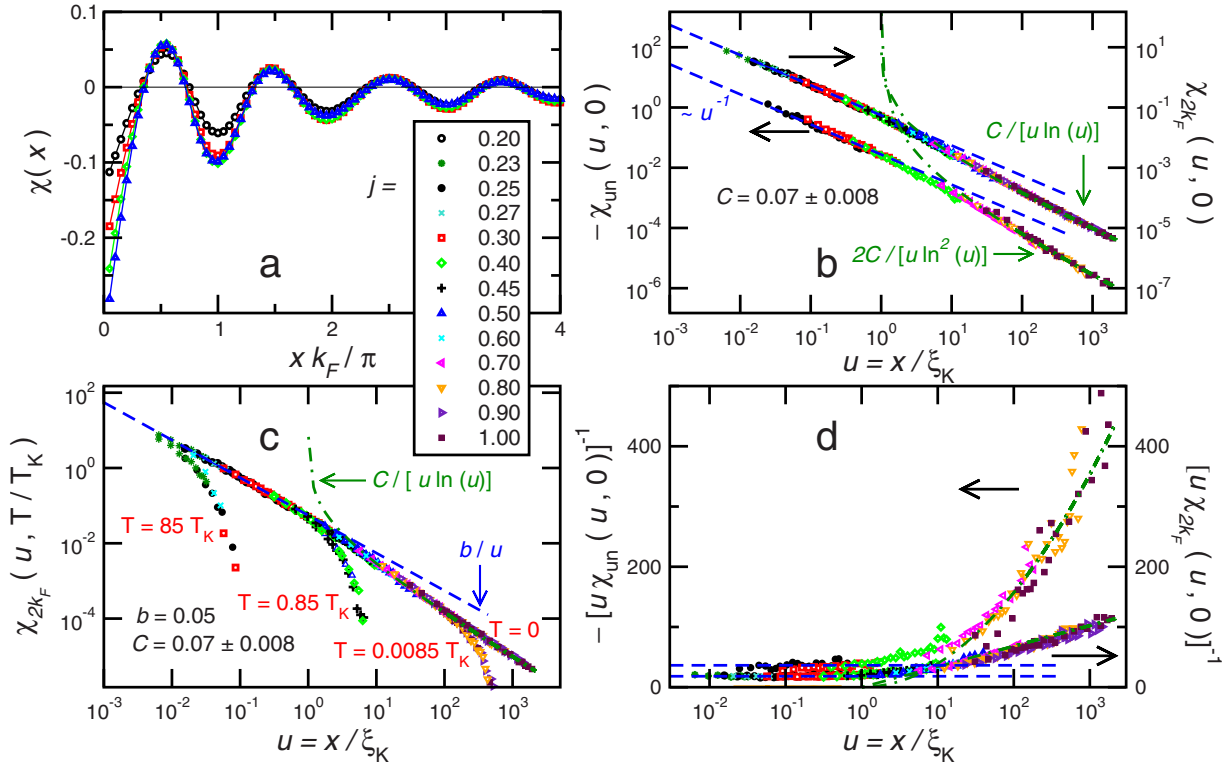
FIG. 1. (Color online) Panel a: the equal-time spin-spin correlation function $\chi(x,T) = \langle \vec{S}_{\mathrm{imp}} \vec{s}(x) \rangle$ as a function of the distance $x$ measured from the $S=1$ impurity for different values of the Kondo coupling $j = \nu J$. Unlike the situation for the completely screened Kondo impurity, $\chi$ changes sign as a function of distance, and the electron-spin density close to $x = (n + \frac{1}{2})\frac{\pi}{k_F}$ is aligned, rather than being anticorrelated, with the impurity spin. In panel b, we show the amplitude of the $2k_F$ oscillating and uniform part of $\chi$ at $T=0$ that are universal functions of $x/\xi_K$ [see Eq. (5)]. While for short distances both functions decay as $\sim x^{-1}$, they both obtain logarithmic corrections for $x > \xi_K$. As shown in panel c, the envelope of the oscillating part crosses over from $\sim x^{-1}$ (dashed line) to $\sim 1/[x \ln(x/\xi_K)]$ (dotted-dashed line) at around the Kondo coherence length $\xi_K$. Any finite temperature introduces another length scale $\xi_T = \hbar v_F/(k_B T)$ at which the envelope function crosses over to an exponential decay. The uniform part decays faster beyond the Kondo coherence length: it tends to zero as $\sim 1/[x \ln^2(x/\xi_K)]$. For better visualization, we plot $1/[x\chi(x)]$ as a function of $x/\xi_K$ in panel d.

quite unlike the situation for the Friedel oscillations:[7] in that case the nonuniversal part of the charge-density oscillations is much more extended in space. The additional factor $1/\xi_K$ in Eq. (5) accounts for the correct dimensional units of $\chi(x,T)$. (Note that $\vec{s}(x)$ is a one-dimensional spin density.) Moreover, we anticipated already the phase shift $\delta_0 = \pi/2$ that the electrons attain from screening of half of the impurity spin-1. In order to identify the two functions $\mathcal{X}_{2k_F}$ and $\mathcal{X}_{\mathrm{un}}$, we independently determined the Kondo temperature $T_K$. This was done by extracting the single-particle phase shifts in the presence of a local magnetic field $B$ directly from the NRG spectra and fitting them to Eq. (2).

The two universal functions $\mathcal{X}_{2k_F}$ and $\mathcal{X}_{\mathrm{un}}$ at zero temperature $T=0$ are shown in Fig. 1(b). Both decay algebraically as $1/x$ supplemented by logarithmic corrections for large distances $x > \xi_K$. In the presence of a finite temperature, the decay changes from algebraic to exponential for $x > \xi_T$, where $\xi_T = \hbar v_F/(k_B T)$ is the thermal length, as it is shown in panel Fig. 1(c) for the amplitude of the oscillating part.

It is expected that the long-distance behavior of $\chi(x,T)$ at $T \ll T_K$ is captured by an effective ferromagnetic spin-$\frac{1}{2}$ Kondo model. Assuming that at large distances $x \gg \xi_K$, the correlator is dominated by the unscreened part of the magnetic moment $S^*_{\mathrm{imp}} = \frac{1}{2}$,

$$\chi(x,T) \sim \langle \vec{S}^*_{\mathrm{imp}} \vec{s}(x) \rangle, \quad \text{for} \quad x \gg \xi_K, \tag{6}$$

we can apply perturbation theory in the effective ferromagnetic coupling $J_{\mathrm{eff}}(\varepsilon)$ to calculate the asymptotic behavior. The amplitude of the $2k_F$ oscillating part starts in the first order and the amplitude of the uniform part in the second order in $J_{\mathrm{eff}}(\varepsilon)$. Its logarithmic energy dependence results in characteristic logarithmic corrections to power-law decay,[3]

$$\chi(x,T=0) = \frac{\mathcal{C}}{x} \left[ \frac{\cos(2k_F x + 2\delta_0)}{\log(x/\xi_K)} - \frac{2}{\log^2(x/\xi_K)} \right], \tag{7}$$

for $x \gg \xi_K$.

Note that the antiferromagnetic correlations of $\chi$ observed at $x = n\pi/k_F$, with integer $n$, is an unambiguous signature of the additional phase shift $\delta_0 = \pi/2$ due to the partial screening of half of the impurity spin-1. The numerical determination of the coefficient $\mathcal{C}$ is handicapped by the fact that the NRG data only yield reliable information on the spatial spin correlations up to $x/\xi_K \sim 10^3$ such that the asymptotic regime is barely reached. In order to compare with Eq. (7) nonetheless, we employ a two-parameter fit. In addition to the parameter $\mathcal{C}$ in Eq. (7), we allow the Kondo temperature extracted from a fit to the leading-logarithmic expression of the

phase shift (2) to vary by an additional constant parameter $\xi_K = \mathcal{A}\hbar v_F/(k_B T_K^{\text{phase shift}})$. Adjusting the parameters $\mathcal{A}$ and $\mathcal{C}$ for a best fit to the long-distance tail, we obtain $\mathcal{C} = 0.07 \pm 0.01$.

Within the numerical accuracy, we find the long-distance tail of $\chi(x,T)$ to be described by a universal coefficient $\mathcal{C}$ in Eq. (7) independent of the Kondo coupling $J$. On the other hand, a renormalization-group treatment of the effective ferromagnetic Kondo model predicts the coefficient $\mathcal{C}$ to depend explicitly on the effective bare ferromagnetic coupling.[3] The numerical finding thus indicates that the low-energy model is characterized by a universal dimensionless ferromagnetic Kondo coupling on the order of 1.

This is borne out by considering the integrated correlator $\chi(T)$ in Eq. (4). At small but finite temperature $T \ll T_K$, the correction $\chi(T) - \chi(0)$ is determined by the long-distance tail of the spin correlator $\chi(x, T=0)$ at *zero* temperature as, effectively, the temperature only cuts off the correlation tail at the distance of the thermal length $\xi_T$. From Eq. (7) we thus obtain the asymptotics

$$\chi(T) - \chi(0) = \frac{4\mathcal{C}}{\log(\xi_T/\xi_K)} \quad \text{for} \quad \xi_T \gg \xi_K. \tag{8}$$

This allows for an alternative determination of the coefficient $\mathcal{C}$ by computing $\chi(T)$ with NRG. The result is shown in Fig. 2. It allows a fit to Eq. (8) over more than seven decades in $\xi_T/\xi_K$ yielding a more accurate value for $\mathcal{C} = 0.066 \pm 0.0015$. Whereas $\mathcal{C}$ is found to be universal, the value $\chi(T=0)$ depends on the Kondo coupling $J$ (not shown).

To summarize, we have demonstrated that the profile of the spatial spin correlations $\chi(x,T)$ around an underscreened spin-1 is markedly different from the one of a fully screened
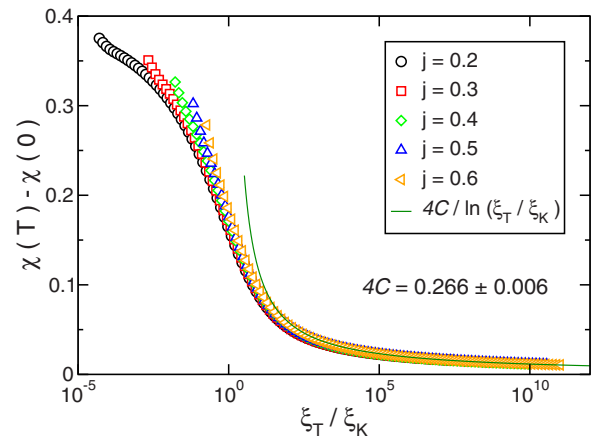


FIG. 2. (Color online) Temperature correction $\chi(T) - \chi(0)$ to the integrated spatial spin correlator (4). At low temperatures $\xi_T \ll \xi_K$, it follows Eq. (8).

spin-$\frac{1}{2}$. The correlations are more pronounced and decay at $T=0$ as $1/x$ in $d=1$ with logarithmic corrections, and they change sign as a function of distance with ferromagnetic correlations at $x k_F / \pi = n + \frac{1}{2}$ with integer $n$. The long-distance behavior is universal and can be explained in terms of an effective ferromagnetic Kondo model.

[1] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, New York, 1993).

[2] H. Ishii, J. Low Temp. Phys. **32**, 457 (1978).

[3] V. Barzykin and I. Affleck, Phys. Rev. B **57**, 432 (1998).

[4] I. Affleck and P. Simon, Phys. Rev. Lett. **86**, 2854 (2001).

[5] E. S. Sørensen and I. Affleck, Phys. Rev. Lett. **94**, 086601 (2005).

[6] L. Borda, Phys. Rev. B **75**, 041307(R) (2007).

[7] I. Affleck, L. Borda, and H. Saleur, Phys. Rev. B **77**, 180404(R) (2008).

[8] P. Mehta, N. Andrei, P. Coleman, L. Borda, and G. Zaránd, Phys. Rev. B **72**, 014430 (2005).

[9] W. Koller, A. C. Hewson, and D. Meyer, Phys. Rev. B **72**, 045117 (2005).

[10] N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).

[11] Ph. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).

[12] O. Újsághy, A. Zawadowski, and B. L. Gyorffy, Phys. Rev. Lett. **76**, 2378 (1996).

[13] R. Žitko, R. Peters, and Th. Pruschke, Phys. Rev. B **78**, 224404 (2008).

[14] M. Pustilnik and L. I. Glazman, Phys. Rev. Lett. **87**, 216601 (2001).

[15] A. Posazhennikova and P. Coleman, Phys. Rev. Lett. **94**, 036802 (2005).

[16] J. B. Silva, W. L. C. Lima, W. C. Oliveira, J. L. N. Mello, L. N. Oliveira, and J. W. Wilkins, Phys. Rev. Lett. **76**, 275 (1996).