Pair-Density-Wave Correlations in the Kondo-Heisenberg Model

Erez Berg,[1] Eduardo Fradkin,[2] and Steven A. Kivelson[3]

[1]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

[2]*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3080, USA*

[3]*Department of Physics, Stanford University, Stanford, California 94305-4060, USA*

(Received 23 April 2010; published 28 September 2010)

We show, using density-matrix renormalization-group calculations complemented by field-theoretic arguments, that the spin-gapped phase of the one dimensional Kondo-Heisenberg model exhibits quasi-long-range superconducting correlations *only* at a nonzero momentum. The local correlations in this phase resemble those of the pair-density-wave state which was recently proposed to describe the phenomenology of the striped ordered high-temperature superconductor $La_{2-x}Ba_xCuO_4$, in which the spin, charge, and superconducting orders are strongly intertwined.

DOI: 10.1103/PhysRevLett.105.146403 PACS numbers: 71.10.Fd, 74.20.−z, 74.72.−h

Recent experiments in the high-temperature superconductor $La_{2-x}Ba_xCuO_4$ near doping $x = 1/8$ have revealed a dramatic layer decoupling effect in which anomalous mesoscopic 2D superconductivity persists well above the macroscopic 3D superconducting transition temperature T_c. [1–3] Moreover, the superconductivity coexists with static stripe (charge and spin) order. It has been proposed that the anomalous superconducting properties are evidence of the existence of a novel type of superconducting state, the pair-density wave (PDW) [4–6].

The PDW is a state in which charge, spin, and superconducting (SC) orders are *intertwined* in a spatially modulated fashion. The SC order has a wave vector $\mathbf{Q}$ which is the same as that of the spin-density wave and half of the ordering wave vector $2\mathbf{Q}$ of the charge-density wave (CDW). Its SC order is Larkin-Ovchinnikov–like, but without the magnetization of the latter. Although much is known about the properties of this state [5,6], there is, as yet, no fully satisfactory microscopic theory.

In the context of Bardeen-Cooper-Schrieffer–type mean-field theories, a PDW is only ever stable at strong coupling [7] (i.e., outside the regime in which such treatments are reliable). Slave-boson mean-field theories of the t-J model find that, although the PDW is quite competitive energetically, it (barely) loses to the uniform d-wave SC state [8]. While early numerical variational Monte Carlo studies of the t-J model found a regime in which the PDW appeared to be stable [9], more recent studies have found that it has slightly higher variational energy than the uniform d-wave state [10,11].

In this Letter we study the superconducting correlations in the 1D Kondo-Heisenberg model (KHM). This is the simplest model in which one can investigate the interplay between strong antiferromagnetic ordering tendencies, represented by a Heisenberg chain, and possible superconducting and charge-density-wave orders, derived from an itinerant electron band to which it is coupled. The 1D character of the model permits us to employ the powerful numerical density-matrix renormalization-group (DMRG) [12] and analytic bosonization methods to solve the problem, despite the strong interactions. On the downside, there are special features of 1D physics, which may raise questions concerning the applicability of the results to higher dimensional situations. On the other hand, especially since the order we are investigating is unidirectional, and thus has an essentially 1D geometry, it is plausible that the local structure of the correlations up to intermediate scales are dimension independent.

The key finding from our DMRG studies is that, for the range of parameters considered here, the 1D KHM exhibits a spin-gapped phase with quasi-long-range (power-law) PDW correlations, i.e., superconducting correlations which oscillate with a period $2b$ where b is the lattice constant of the Heisenberg chain. At the same time the uniform singlet superconducting correlations are small and apparently fall exponentially with distance. Since the same model exhibits substantial, although short-ranged correlated, antiferromagnetic tendencies with the same period, this state can clearly be identified as a fluctuating version of the long-sought PDW. Note that the occurrence of a spin gap in the 1D Kondo-Heisenberg model has been discussed insightfully in the literature [13,14], and the possibility of an oscillatory superconducting order parameter was previously inferred on the basis of bosonization studies [15–20]. However, we believe that this is the first place in which the existence and character of this state has been derived from a microscopic model and the nature of the correlations is elucidated [21].

Model.—The 1D KHM is defined as a one dimensional electron gas (1DEG) coupled to a spin-$\frac{1}{2}$ chain:

$$H = H_{1\mathrm{DEG}} + H_{\mathrm{Heis}} + H_K, \tag{1}$$

where

$$H_{1\mathrm{DEG}} = -t\sum_{j,\sigma} c^\dagger_{j\sigma} c_{j+1\sigma} + \mathrm{H.c.} - \mu \sum_{j,\sigma} n_j, \tag{2}$$

 © 2010 The American Physical Society

$$H_{\mathrm{Heis}} = J_H \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \tag{3}$$

$$H_K = J_K \sum_{j,a} S_j^a [c_{j\sigma}^\dagger (s^a)_{\sigma\sigma'} c_{j\sigma'}]. \tag{4}$$

Here, $c_{j\sigma}^\dagger$ creates an electron with spin σ at site j, $\mathbf{S}_j$ is the spin-$\frac{1}{2}$ operator of the spin chain, and $s^a = \frac{1}{2}\tau^a$ ($\tau^{a=x,y,z}$ are Pauli matrices).

In typical physical circumstances in which Kondo physics arises, one would expect J_H and $J_K \ll t$. In this limit, the length scales characterizing the Kondo effect are exponentially large, and hence not readily accessible by any numerical method. We therefore use $J_H \sim J_K \sim t$. On the basis of the field-theoretic analysis (see below), we expect the character of the phases to survive to small J/t. Moreover, the $J_H \sim J_K \sim t$ regime is not necessarily unphysical; it can be derived from the $U \to \infty$ limit of a Hubbard model on the spin chain, with chemical potential chosen so that there is one electron per site, and with hopping matrix element along the chain, $t_H = \sqrt{J_H U/2}$, and hopping between the spin chain and the 1DEG, $t_K = \sqrt{J_K U/2}$.

Numerical results.—The model (1) was solved using DMRG on finite lattices with $L = 32$–128 and open boundary conditions. Up to $m = 1800$ states were kept, giving DMRG truncation errors smaller than 10^{-6}.

Figure 1 shows the spin gap $\Delta_s = E_0(1) - E_0(0)$, where $E_0(S_z)$ is the ground state energy of a system with a z spin projection S_z. The spin gap was extrapolated to the thermodynamic ($L \to \infty$) limit. The results are shown for $J_H = J_K = 2t$, as a function of the concentration of electrons in the 1DEG, n. Because of the particle-hole symmetry of the model, it is sufficient to consider $n < 1$.

Near $n = 1$ there is a sizable spin gap [14]; Δ_s decreases away from $n = 1$. For $n = 1$ (not shown), the spin gap is $\Delta_s \approx 0.8$, but there is also a finite charge gap in the $L \to \infty$ limit. We henceforth focus on $n = 0.875$, for which Δ_s is substantial. Since Δ_s persists at lower densities, we expect the low-energy properties at smaller n to be similar, although the correlation length is larger.

PDW correlations.—The opening of a spin gap is expected to lead to enhanced SC (as well as CDW) correlations. To study these correlations, we have applied a local pair field to the left boundary [22]:

$$H_{\mathrm{pair}} = \Delta(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger) + \mathrm{H.c.}, \tag{5}$$

where we fixed $\Delta = 0.5t$. (We have checked explicitly that the results do not depend on the size of Δ [23].) The superconducting response of the system was probed by measuring the following induced order parameters throughout the system [24]:

$$\phi(j) = \langle c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle, \qquad \phi_B(j) = \frac{1}{2}\langle c_{j\uparrow}^\dagger c_{j+1\downarrow}^\dagger - c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger \rangle, \tag{6}$$

where $\phi(j)$ and $\phi_B(j)$ are, respectively, the expectation of the singlet pair creation operator on site j and on the bond from site j to site $j+1$. Figure 2(a) shows $\phi(j)$ and $\phi_B(j)$ in an $L = 64$ system. $\phi(j)$ appears to decay very rapidly away from the left boundary. $\phi_B(j)$ decays much more slowly, and exhibits pronounced oscillations as a function of position with wave vector $q = \pi/b$, as it changes its sign between every consecutive bond. Longer periods are also apparent in the figure. These oscillations clearly indicate that the dominant pairing correlations are at a nonzero momentum.

References [15–17,19,20] proposed, based on bosonization, that the spin-gapped phase of the KHM has dominant pairing correlations at a nonzero wave vector, described by a "composite" order parameter [20]

$$\phi_c(j) = (-1)^j \left\langle \left[\sum_{\sigma,\sigma'} c_{j-1\sigma}^\dagger (is^y \mathbf{s})_{\sigma\sigma'} c_{j+1\sigma'}^\dagger \right] \cdot \mathbf{S}_j \right\rangle. \tag{7}$$

In addition, PDW order should be accompanied by a uniform ($q = 0$) "charge $4e$" order parameter [26]:

$$\phi_{4e}(j) = \langle c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger c_{j+1\downarrow}^\dagger \rangle. \tag{8}$$

Figure 2(b) shows $\phi_{\mathrm{PDW}}(j) \equiv (-1)^j \phi_B(j)$, as well as $\phi_c(j)$ and $\phi_{4e}(j)$, as a function of position, on a logarithmic scale. The largest, and most slowly decaying, order parameter is $\phi_{\mathrm{PDW}}(j)$, suggesting that the system is best described as a fluctuating PDW state. As expected, $\phi_{4e}(j)$ and $\phi_c(j)$ are nonzero, but small. $\phi_c(j)$ is modulated as a function of position, while $\phi_{4e}(j)$ is smooth.

The wave vectors of the leading SC and CDW fluctuations can be determined by a Fourier analysis of the SC and CDW orders [25]. Figure 3 shows the absolute values of the

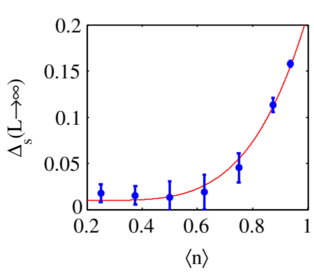

FIG. 1 (color online). Δ_s versus the electron concentration in the 1DEG. $J_H = J_K = 2t$. The error bars are a result of the extrapolation to the thermodynamic limit. (Relative to the extrapolation error, the DMRG truncation error is negligible.)

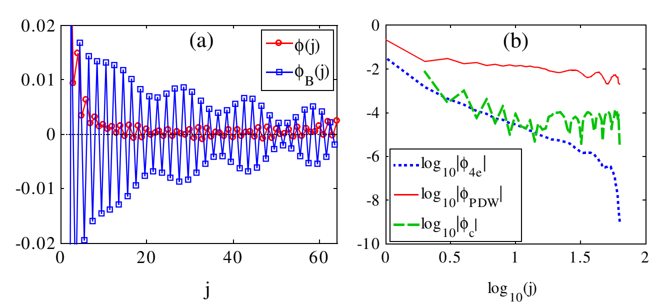

FIG. 2 (color online). (a) The SC order parameters ϕ and ϕ_B (see text) as a function of position in an $L = 64$ system with $n = 0.875$. (b) Measurements of ϕ_{PDW}, ϕ_{4e}, ϕ_c versus position. The oscillatory behavior close to the right boundary is an edge effect.

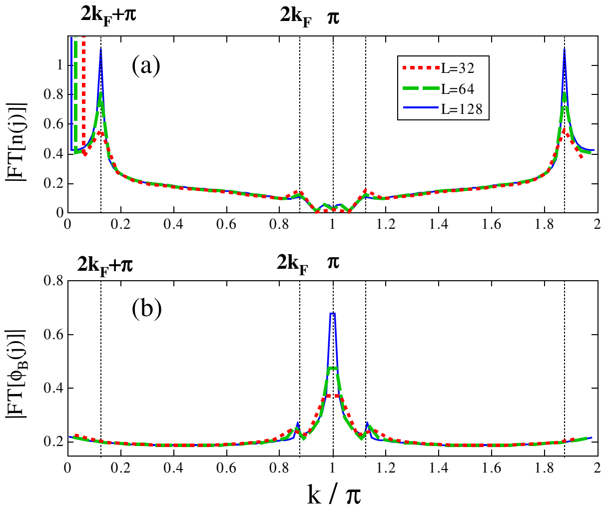

FIG. 3 (color online). Absolute values of the Fourier transforms (FT) of (a) the charge $[\langle n(j)\rangle]$ and (b) the SC $[\phi_B(j)]$ orders. $L = 32$–128.

Fourier transforms of $\phi_B(j)$ and $n(j) \equiv \sum_\sigma c^\dagger_{j\sigma} c_{j\sigma}$ for system sizes between $L = 32$ and 128. The charge density exhibits a large peak at $q = 2k_F + \pi/b$ which grows as a function of system size, where $2k_F \equiv \pi n$. There are also small subleading features at $q = 2k_F$ and $q = \pi/b$. The main feature in the Fourier transform of ϕ_B is a pronounced peak at $q = \pi/b$, with a subleading peak at $q = 2k_F$. This shows unambiguously that the dominant order in this system is a PDW with $q = \pi/b$, accompanied by CDW correlations at $q = 2k_F + \pi/b$.

In order to elucidate further the nature of the microscopic correlations in the system, we perform another simulation in which both a pair field [Eq. (5)] and a Zeeman field, $H_Z = -hS^z_{j=1}$ ($h = 0.5t$), are applied to the left boundary of the system. The induced charge, superconducting, and magnetic ($\langle S^z_j\rangle$) order parameters are shown near the middle of the $L = 64$ system in Fig. 4(a). The magnetic order oscillates at wave vector $q = \pi/b$ (the same as the PDW) with an envelope that decays exponentially on longer length scales.

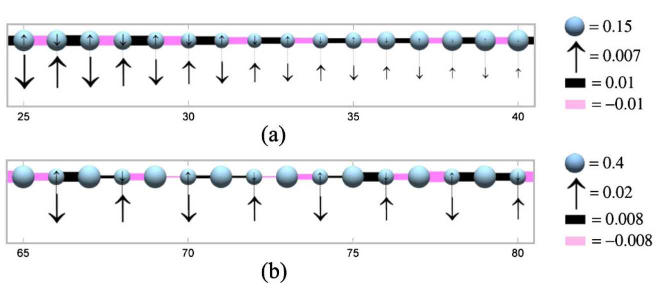

FIG. 4 (color online). Order parameters in (a) an $L = 64$ KHM chain with $n = 0.875$ and (b) an $L = 128$ "diluted" KHM chain (with one spin site for each two 1DEG sites) with $n = 0.625$. Circles, 1DEG hole density $[1 - \langle n(j)\rangle]$; bond color and thickness, the bond-centered SC amplitude $\phi_B(j)$. The arrows show the spin density $\langle S^z(j)\rangle$.

Next, we would like to understand what determines the PDW wave vector. We performed another calculation in which the spin chain is "diluted"; i.e., there is one spin site for every *two* 1DEG sites. Equation (3) is replaced by $\tilde{H}_{\rm Heis} = J_H \sum_j \mathbf{S}_{2j} \cdot \mathbf{S}_{2j+2}$, and similarly $\tilde{H}_K = J_K \sum_{j,a} S^a_{2j} [c^\dagger_{2j\sigma}(s^a)_{\sigma\sigma'} c_{2j\sigma'}]$. Figure 4(b) illustrates the results for $\langle S^z_j\rangle$, $\langle n_j\rangle$, and ϕ_B near the middle of an $L = 128$ system. (In order to maintain a large spin gap, n was taken to be 0.625.) Clearly, the PDW order changes sign across every spin site, indicating that the dominant PDW wave vector is again $q = \pi/b$, where now $b = 2$. Thus, the period of the PDW is tied to that of the local (fluctuating) magnetic ordering. The local correlations in Figs. 4(a) and 4(b) are a one dimensional version of the phenomenologically proposed "striped-superconducting" state for $La_{2-x}Ba_xCuO_4$ [4].

Continuum limit.—Analytical progress can be made in the limit $J_H, t \gg J_K$, where we may first take the continuum limit of both the 1DEG and the spin chain. We use a description in terms of the bosonic fields φ_c, φ_s, and $\tilde{\varphi}_s$, representing charge or spin fluctuations in the 1DEG and spin chain, respectively (and the respective conjugate fields θ_c, θ_s, and $\tilde{\theta}_s$). The Hamiltonian densities of the 1DEG and the spin chains take the form [13,19,20]

$$\mathcal{H}_{\rm 1DEG} = \sum_{\alpha=c,s} v_\alpha \left[\frac{K_\alpha}{2} (\partial_x \theta_\alpha)^2 + \frac{1}{2K_\alpha} (\partial_x \varphi_\alpha)^2 \right],$$
$$\mathcal{H}_{\rm Heis} = \frac{1}{2} \tilde{v}_s [(\partial_x \tilde{\theta}_s)^2 + (\partial_x \tilde{\varphi}_s)^2], \qquad (9)$$

where K_c, K_s, v_c, v_s, and $\tilde{v}_s$ are, respectively, the charge and spin Luttinger parameters of the 1DEG and the corresponding charge and spin velocities. The various bosonized fields satisfy the commutation relation $[\varphi_\alpha(x), \partial_x \theta_\alpha(x')] = i\delta(x - x')$, and similarly for $\tilde{\theta}_s$, $\tilde{\varphi}_s$. We neglect marginally irrelevant contributions to $H_{\rm Heis}$.

For a an incommensurate filling n of the 1DEG, only "forward scattering" terms in the spin channel can couple the 1DEG and the spin chain. Up to irrelevant (backscattering) operators, the Kondo Hamiltonian density is $\mathcal{H}_K = \frac{J_K a}{8\pi} [(\partial_x \varphi_+)^2 - (\partial_x \varphi_-)^2] + \mathcal{H}_{\rm int}$ [13], where $\theta_\pm = \frac{1}{\sqrt{2}} (\tilde{\theta}_s \pm \theta_s)$, $\varphi_\pm = \frac{1}{\sqrt{2}} (\tilde{\varphi}_s \pm \varphi_s)$, and $\mathcal{H}_{\rm int} = \frac{\cos(\sqrt{4\pi}\theta_-)}{2(\pi a)^2} [\cos(\sqrt{4\pi}\varphi_-) + \cos(\sqrt{4\pi}\varphi_+)]$. ($a$ is a microscopic cutoff.) Under renormalization, $\cos(\sqrt{4\pi}\theta_-) \times \cos(\sqrt{4\pi}\varphi_+)$ is marginally relevant [13], while $\cos(\sqrt{4\pi}\theta_-) \cos(\sqrt{4\pi}\varphi_-)$ is irrelevant, since it contains the dual fields θ_- and φ_-. The strong coupling phase has a spin gap, while the charge degree of freedom φ_c remains decoupled and gapless.

Correlations in the spin-gapped phase.—The form of the dominant (slowest decaying) correlations follows from the following considerations. A theorem by Yamanaka *et al.* [27] guarantees the existence of a charge zero, momentum $2k^*_F = \pi n_{\rm tot}$ gapless excitation, where $n_{\rm tot}$ is the total electron density in the system (counting both the 1DEG and the spin chain). Here, $n_{\rm tot} = n + \frac{1}{b}$; therefore,

$2k_F^* = 2k_F + \pi/b$. Let us denote the operator that creates these excitations $\hat{O}_{2k_F^*}$. Since there is a spin gap, $\hat{O}_{2k_F^*}$ is necessarily a spin singlet, i.e., a CDW operator.

In addition, as long as there is no charge gap, the singlet "η-pairing operator" [16,20] $\hat{O}_\eta = \psi_{-\uparrow}\psi_{-\downarrow} = \frac{1}{2\pi a} \times \exp[i\sqrt{2\pi}(\theta_c - \phi_c)]$ also creates gapless excitations. [$\psi_{\pm,\sigma}$ annihilate right- (left-)moving electrons with spin $\sigma = \uparrow, \downarrow$, respectively.] This operator has total momentum $-2k_F$ and charge $2e$. Therefore, the "PDW operator" $\hat{O}_{\mathrm{PDW}} = \hat{O}_\eta \hat{O}_{2k_F^*}$ also creates gapless excitations. Adding the quantum numbers carried by $\hat{O}_\eta$ and $\hat{O}_{2k_F^*}$, we see that $\hat{O}_{\mathrm{PDW}}$ carries charge $2e$ and momentum π/b. This guarantees the existence of quasi-long-range PDW correlations in the spin-gapped phase. As usual, the correlations of $\hat{O}_{\mathrm{PDW}}$ (as well as those of $\hat{O}_{2k_F^*}$) fall off with a nonuniversal exponent, which depends on K_c. The (zero momentum) Cooper pair operator is $\hat{O}_{\mathrm{SC}} = \psi_{+\uparrow}\psi_{-\downarrow} = \frac{1}{2\pi a} e^{i\sqrt{2\pi}(\theta_c + \phi_s)}$. Its correlations are short ranged, since $\phi_s = (\phi_+ + \phi_-)/\sqrt{2}$; in the spin-gapped phase the field θ_- is pinned, while its dual ϕ_- undergoes strong fluctuations, suppressing the correlations of $\hat{O}_{\mathrm{SC}}$. Consequently, the leading superconducting correlations are for operators with nonzero momentum.

Generically, any singlet operator that carries charge $2e$ and momentum π/b is expected to couple to $\hat{O}_{\mathrm{PDW}}$, and therefore to have quasi-long-range correlations. For example, both ϕ_{PDW} and ϕ_c defined above have the correct quantum numbers, and therefore their correlations should fall off with the same exponent as that of $\hat{O}_{\mathrm{PDW}}$. According to our numerical simulations, the spin-gapped phase has strong PDW correlations, so it is best characterized by the ϕ_{PDW} order parameter. The results in Fig. 3 are fully consistent with the field-theoretic analysis above. In particular, the density profile shows a large peak at $q = 2k_F^*$ which grows with system size, indicating slowly decaying fluctuations centered at that wave vector. The pairing correlations are strongly peaked at $q = \pi/b$, with a subdominant peak (which does not grow with L) at $q = 2k_F$, corresponding to the gapless η-pairing mode.

Discussion.—The correlations in the spin-gapped phase of the 1D KHM are best described as a PDW phase, which is a (quasi)condensate of nonzero center of mass momentum Cooper pairs. Locally, the correlations are strikingly similar to those of the PDW state recently proposed to describe the striped phase of $La_{2-x}Ba_xCuO_4$, which intertwines spin, charge, and density orders. A study of a two-chain KHM found, instead, dominant uniform pairing correlations [28]. It remains an important question whether the PDW state survives in other multichain generalizations of the present model. Finally, the 1D KHM can be viewed as a variation of the three-band copper-oxide model [29], with strongly localized spins on the Cu sites and a 1DEG representing doped holes on O sites. Therefore it seems plausible that such a model can exhibit a PDW phase as well. Whether it can be realized in the physically relevant parameter regime remains to be seen.

We thank P. Coleman, T. Giamarchi, A. Tsvelik, and S. White for discussions. We thank the KITP at UCSB for hospitality. This work was supported in part by the NSF, under Grants No. DMR-0758462 (E. F.), No. DMR-0531196 (S. A. K.), No. DMR-0705472 and No. DMR-0757145 (E. B.), and No. PHY05-51164 at KITP (E. B., E. F., S. A. K.), and by the DOE under Contracts No. DE-FG02-07ER46453 at UIUC (E. F.) and No. DE-FG02-06ER46287 at Stanford (S. A. K.).

[1] Q. Li *et al.*, Phys. Rev. Lett. **99**, 067001 (2007).
[2] J. Tranquada *et al.*, Phys. Rev. B **78**, 174529 (2008).
[3] A. A. Schafgans *et al.*, Phys. Rev. Lett. **104**, 157002 (2010).
[4] E. Berg *et al.*, Phys. Rev. Lett. **99**, 127003 (2007).
[5] E. Berg, E. Fradkin, and S. A. Kivelson, Phys. Rev. B **79**, 064515 (2009).
[6] E. Berg *et al.*, New J. Phys. **11**, 115004 (2009).
[7] F. Loder, A. P. Kampf, and T. Kopp, Phys. Rev. B **81**, 020511(R) (2010).
[8] K.-Y. Yang *et al.*, New J. Phys. **11**, 055053 (2009).
[9] A. Himeda, T. Kato, and M. Ogata, Phys. Rev. Lett. **88**, 117001 (2002).
[10] M. Raczkowski *et al.*, Phys. Rev. B **76**, 140505(R) (2007).
[11] M. Capello, M. Raczkowski, and D. Poilblanc, Phys. Rev. B **77**, 224502 (2008).
[12] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[13] S. R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996).
[14] A. E. Sikkema, I. Affleck, and S. R. White, Phys. Rev. Lett. **79**, 929 (1997).
[15] O. Zachar, S. A. Kivelson, and V. J. Emery, Phys. Rev. Lett. **77**, 1342 (1996).
[16] V. J. Emery, S. A. Kivelson, and O. Zachar, Phys. Rev. B **59**, 15 641 (1999).
[17] P. Coleman *et al.*, Phys. Rev. B **60**, 3608 (1999).
[18] J. Moreno *et al.*, Phys. Rev. B **64**, 085116 (2001).
[19] O. Zachar and A. M. Tsvelik, Phys. Rev. B **64**, 033103 (2001).
[20] O. Zachar, Phys. Rev. B **63**, 205104 (2001).
[21] A related model, with the 1DEG replaced by a t-J chain and an anisotropic J_K, was studied by K. A. Al-Hassanieh *et al.*, Phys. Rev. B **80**, 115116 (2009).
[22] A. E. Feiguin *et al.*, Phys. Rev. Lett. **101**, 217001 (2008).
[23] See supplementary material at http://link.aps.org/supplemental/10.1103/PhysRevLett.105.146403 for additional numerical results.
[24] Applying boundary fields and measuring the response is qualitatively similar to measuring two-point correlations. However, the exponent with which the correlations decay can be different in the two cases. See, e.g., [25].
[25] The charge density is nonuniform due to the presence of the boundaries; see S. R. White, I. Affleck, and D. J. Scalapino, Phys. Rev. B **65**, 165122 (2002).
[26] E. Berg, E. Fradkin, and S. A. Kivelson, Nature Phys. **5**, 830 (2009).
[27] M. Yamanaka, M. Oshikawa, and I. Affleck, Phys. Rev. Lett. **79**, 1110 (1997).
[28] J. C. Xavier and E. Dagotto, Phys. Rev. Lett. **100**, 146403 (2008).
[29] V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).