Incoherent transport induced by a single static impurity in a Heisenberg chain

O. S. Barišić,[1,2] P. Prelovšek,[1,3] A. Metavitsiadis,[4] and X. Zotos[4]
[1]*J. Stefan Institute, SI-1000 Ljubljana, Slovenia*
[2]*Institute of Physics, HR-10000 Zagreb, Croatia*
[3]*Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia*
[4]*Department of Physics, Foundation for Research and Technology-Hellas, University of Crete, P.O. Box 2208, 71003 Heraklion, Greece*
(Received 25 August 2009; published 18 September 2009)

The effect of a single static impurity on the many-body states and on the spin and thermal transport in the one-dimensional anisotropic Heisenberg chain at finite temperatures is studied. Whereas the pure Heisenberg model reveals Poisson level statistics and dissipationless transport due to integrability, we show using the numerical approach that a single impurity induces Wigner-Dyson level statistics and at high enough temperature incoherent transport within the chain, whereby the relaxation time and dc conductivity scale linearly with length.

DOI: 10.1103/PhysRevB.80.125118 PACS number(s): 71.27.+a, 71.10.Pm, 72.10.−d

Transport in the one-dimensional (1D) quantum system of interacting particles still offers several fundamental theoretical challenges. In the context of the electron transport through barriers or weak links the role of repulsive electron-electron interactions within the wire was shown to be crucial[1,2] since at low temperature $T\to 0$ the interaction within Luttinger-liquid (LL) phenomenology renormalizes the transmission through the barrier to zero effectively cutting the chain for transport.[3] Neglecting the effect of umklapp processes within the wire above the Kane-Fisher temperature T^* the transmission through the barrier should become finite[1,2] indirectly confirmed in a numerical study of the 1D spin model.[4] On the other hand, in the last decade it has become increasingly evident that the LL low-energy description is not enough to establish transport properties, if they are dominated by umklapp processes. It has been shown[5,6] that pure 1D integrable models of interacting fermions exhibit in spite of umklapp at any $T>0$ dissipationless (ballistic) transport manifested, e.g., in a finite charge stiffness $D(T>0)>0$. On contrary, a generic system of interacting fermions would exhibit dissipation in the wire and also finite dc transport coefficients, e.g., the dc conductivity $\sigma(\omega\to 0)=\sigma_0<\infty$. The distinction is closely linked to the statistics of many-body levels,[7] which follow the Poisson level distribution for the integrable system and the Wigner-Dyson (WD) distribution for the generic nonintegrable system.[5] Random disorder, strong enough to overcome finite-size effects, in such models generally leads to the WD statistics for nearest levels,[8,9] while the dc transport seems to be normal (dissipative) at $T>0$,[10] in contrast to the Anderson-type localization persisting at $T=0$.[11]

Our goal is to understand within this context the effect of a single static impurity in the 1D integrable system of interacting particles. While of fundamental importance this question is also directly relevant in connection with ongoing experiments on novel quasi-1D materials where electronic properties of the pure system can be well described within the integrable spin-1/2 Heisenberg model[12] with dilute impurities introduced in a controlled manner and their influence studied, e.g., on the thermal transport.

In the following we show on the example of the 1D spin model with periodic boundary conditions that a single static impurity can qualitatively change the level statistics to the WD one, noticed also in the recent study of the onset of quantum chaos[13] although the perturbation scales as $1/L$ where L is the length of the system. At the same time, the impurity leads to the vanishing of the spin stiffness D at elevated $T>0$. In such a situation, it is meaningful to discuss the decay of the spin and energy current within the ring and related transport rates $1/\tau$ which we show to be well defined and scale as $1/\tau\propto 1/L$ as expected for the homogeneous wire with a single localized perturbed region.

We consider the 1D anisotropic Heisenberg model (AHM) with a single-site static impurity field,

$$H=\sum_l J(S^x_{l+1}S^x_l+S^y_{l+1}S^y_l+\Delta S^z_{l+1}S^z_l)+b_0S^z_0, \qquad (1)$$

where $S^\alpha, \alpha=x,y,z$ are spin-1/2 operators, J is the magnetic exchange coupling (we use units $J=1$), Δ the anisotropy, and b_0 the local impurity field. Numerically we study chain (ring) of length L with periodic boundary conditions.

In the absence of the impurity the AHM, Eq. (1), is integrable and as the consequence reveals the Poisson level distribution $P_P(s)=\exp(-s)$ where $s=(E_{n+1}-E_n)/\Delta_0$ (Δ_0 is the average level spacing) as well as the dissipationless transport.[6] Let us first consider the effect of finite b_0 on the level statistics. We investigate this question by performing the (full) exact-diagonalization (ED) study of finite-size systems with $L=10-16$. It should be pointed that in this range the number of many-body states varies (in the $S^z_{tot}=0$ sector) in a wide range $N_{st}=10^2-10^4$ and the corresponding $\Delta_0=2\times 10^{-2}-5\times 10^{-4}$. The general conclusion is that finite $b_0>0$ induces WD distribution $P_{WD}(s)=(\pi s/2)\exp(-\pi s^2/4)$ following the random-matrix theory (RMT) (Ref. 7) in spite of the fact that the perturbation is only an $1/L$ effect (the perturbation $b_0/2$ relative to the full energy span $\Delta_E\sim LJ$).

To be concrete we present here two standard tests for the closeness of the RMT. The first one is parameter η (Ref. 8) measuring the normalized distance to the WD distribution,

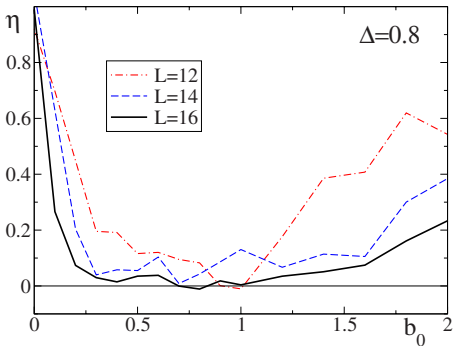

FIG. 1. (Color online) Parameter η for the deviation from the WD level distribution vs impurity field b_0 for $\Delta=0.8$ and various L.

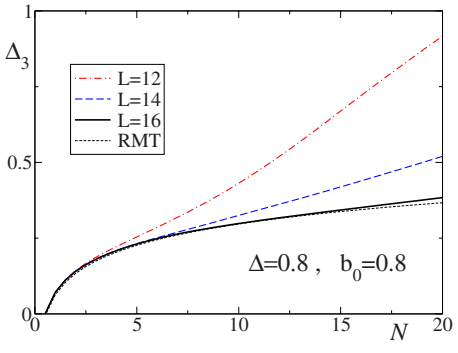

FIG. 2. (Color online) Level-fluctuation parameter $\Delta_3(N)$ for fixed $\Delta=0.8$ and $b_0=0.8$ and different system length L. For comparison the RMT result is presented (dotted line).

$$\eta = \int_0^{s_0} [P(s) - P_{WD}(s)]ds / \int_0^{s_0} [P_P(s) - P_{WD}(s)]ds, \quad (2)$$

where $P(s)$ is the actual level distribution and $s_0=0.473$ is chosen to be the intersection of $P_P(s)$ and $P_{WD}(s)$.[8] In order to stay within the regime of homogeneous density of states we analyze only one half of intermediate many-body states, as relevant for the high-T properties discussed here. ED results for resulting η as a function of b_0 for chosen intermediate $\Delta=0.8$ are presented for different L. To avoid the effect of higher degeneracy of levels at $S^z_{tot}=0, b_0=0$ presented results in Fig. 1 are for $S^z_{tot}=1$. In the absence of impurity ($b_0=0$) we obtain $\eta=1$ since $P(s)=P_P(s)$ due to the integrability of the pure AHM. The most important conclusion is that rather weak impurity $b_0 \sim 0.2$ in largest $L=16$ causes a fast drop to $\eta \sim 0$, i.e., to $P(s) \sim P_{WD}(s)$, whereby the threshold value of b_0 is decreasing with L so that for largest $L=16$ reachable with ED we get $P(s) \sim P_{WD}(s)$ in the range $0.2 < b_0 < 1.5$. On the other side, it is quite remarkable that η starts to recover toward $\eta \sim 1$ again for large $b_0 \gg 1$. This can be easily explained by noting that large $|b_0| \gg 1$ effectively cut the ring and lead to the AHM with open ends which is again an integrable model.

Even stronger probe of the level statistics is the correlation Δ_3 measuring the level fluctuations beyond the nearest neighbor levels,[7]

$$\Delta_3 = \frac{1}{2N} \min_{A,B} \int_{-N}^{N} [\mathcal{N}(\tilde{E}) - A\tilde{E} - B]^2 d\tilde{E}, \quad (3)$$

where $\mathcal{N}(\tilde{E})$ is the integrated density of states with $\tilde{E}=E/\Delta_0$.[14] Δ_3 should behave as $\Delta_3 \sim N/15$ for Poisson distribution, and asymptotically as $\Delta_3 \sim (\ln N)/\pi^2$ within the RMT.[7] In Fig. 2 we present results for $\Delta_3(N)$ for fixed $\Delta=0.8$ and $b_0=0.8$ as obtained for different $L=12-16$. A comparison with the result expected from the RMT shows that $\Delta_3(N)$ approaches the latter very accurately in an interval $N < N^*(L)$ with N^* strongly (exponentially) increasing with L, while the deviation into a Poisson-like linear dependence $\Delta_3 \propto N$ appears for $N > N^*(L)$. Such a generic crossover has been observed also in other systems[15] and one can discuss the relevance of the related crossover energy scale $\epsilon = N^* \Delta_0$. Fast increase in $N^*(L)$ one can understand by noting that the impurity perturbation being L independent mixes up many-body levels[8] within the interval ϵ whereby separation between many-body levels decreases as $\Delta_0 \propto \exp(-L)$. We can estimate $\epsilon \sim b_0/(4L)$ within the XY ($\Delta=0$) model which gives right order of magnitude for observed N^* in Fig. 2. More detailed analysis in analogy to other systems[8] is difficult due to the complicated nature of states at intermediate Δ.

Closely related to the onset of the WD distribution by a single impurity is the vanishing of the $T>0$ coherent (ballistic) transport characteristic for integrable systems.[5,6] The measure of the coherent (dissipationless) component for the spin transport is the spin stiffness $D(T)$ (equivalent to the charge stiffness for the related fermionic model). It can be defined via the gauge phase ϕ into the spin-flip terms in Eq. (1), as $\exp(i\phi)S^+_{l+1}S^-_l + \exp(-i\phi)S^-_{l+1}S^+_l$. At finite $T>0$ the spin stiffness can be expressed as

$$D = \frac{1}{2L} \sum_n p_n \frac{\partial^2 \epsilon_n(\phi)}{\partial \phi^2} \sim \frac{\beta}{2L} \sum_n p_n \left(\frac{\partial \epsilon_n(\phi)}{\partial \phi} \right)^2, \quad (4)$$

where $p_n = \exp(-\beta\epsilon_n)/Z$ with $Z = \Sigma_n \exp(-\beta\epsilon_n)$, and the last relation becomes an equality provided that the susceptibility for persistent current vanishes (for finite systems at large enough T). On the other hand, D still depends on the value ϕ where derivatives in Eq. (4) are taken. For the XY model at $\Delta=0$ corresponding via the Wigner-Jordan transformation to tight-binding noninteracting fermions with $t=J/2$ and a potential impurity $\epsilon_0=b_0/2$ one can establish the relation with the transmission through the barrier, as used also in connection with the evaluation of the 1D conductance[16] at $T=0$. For general $T>0$ one gets in the case of NI fermions and $L \to \infty$,

$$D = \frac{\beta}{2L} \sum_k f_k(1-f_k)(v_k)^2 g_k. \quad (5)$$

where $v_k = 2t \sin k$, f_k is the Fermi function with $\mu=0$ for half-filling ($S^z_{tot}=0$) and

$$g_k = \frac{|t_k|^2 \sin^2(L\phi)}{1 - |t_k|^2 \cos^2(L\phi)}, \quad |t_k|^2 = \frac{4t^2 \sin^2 k}{4t^2 \sin^2 k + \epsilon_0^2}. \quad (6)$$

Numerically we recover the behavior $D(\phi)$ as follows from Eqs. (5) and (6) for arbitrary b_0 as far as $\Delta \to 0$. For $\Delta > 0$ the

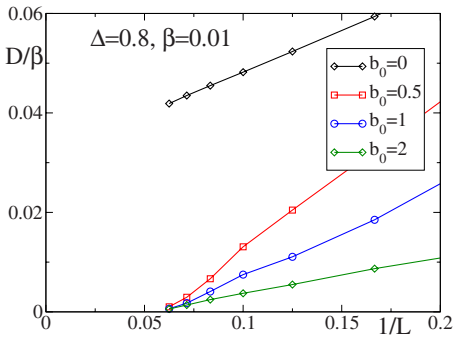

FIG. 3. (Color online) High-T spin stiffness D/β vs $1/L$.

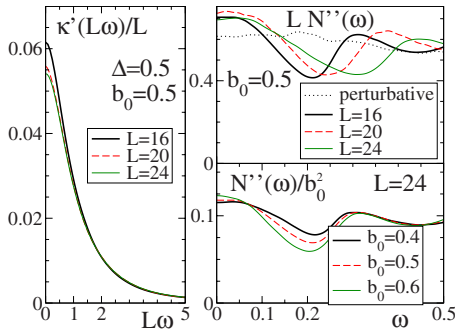

FIG. 4. (Color online) (a) High-T results for scaled thermal conductivity κ'/L vs $L\omega$ for $\Delta=0.5$ and $b_0=0.5$ as calculated for different $L=16-24$. (b) Extracted scaled memory function $LN''(\omega)$. Perturbation-theory result is also plotted (dashed curve). (c) $N''(\omega)/b_0^2$ for different impurity fields $b_0=0.4-0.6$ with $\Delta=0.5$ and $L=24$.

dependence on ϕ remains qualitatively similar, although irregular due to strong dependence on L. In the following we calculate $D(L)$ for fixed $\phi=\pi/(2L)$. Results for $\Delta>0$ are nontrivial for any T. Since results of full ED are best at high T, we restrict ourselves here to the limit $\beta\to 0$. It has been shown for the pure model that D/β remains finite and nontrivial in the thermodynamic limit $L\to\infty$ due to integrability of the model.[6]

In Fig. 3 we show results for D/β vs $1/L$ for chosen $\Delta=0.8$ and for four cases $b_0=0,0.5,1,2$. It is evident from Fig. 3 that $b_0>0$ cases are qualitatively different from the $b_0=0$ where D scales linearly in $1/L$ toward a finite $D/\beta\sim 0.035$. In contrast, $b_0>0$ induces an exponential-like decay of $D\to 0$, at least for large enough $L>L^*$. This is closely related to the onset of the WD distribution and the effective breaking of the integrability. Here, L^* is presumably related to the transport mean-free path, on the other hand such an interpretation is not straightforward. We expect that the exponential decay is generic for any finite $b_0>0$ although it would be difficult to establish numerically for weak b_0 due to L^* increasing beyond available system sizes L.

Rapid (exponential) vanishing of $D(L\to\infty)$ at $T>0$ is the indication that the transport is not ballistic and becomes incoherent (resistive) beyond the characteristic L^*. In order to test this directly we evaluate dynamical spin conductivity $\sigma(\omega)=i[\chi^0_{jj}-\chi_{jj}(\omega)]/\omega^+L$ as well as the related thermal conductivity $\kappa(\omega)=i\beta[\chi^0_{j_Ej_E}-\chi_{j_Ej_E}(\omega)]/\omega^+L$, where j and j_E are spin and energy current, respectively, with corresponding susceptibilities $\chi_{jj}(\omega)=i\int dt e^{i\omega^+t}\langle[j(t),j]\rangle$, and analogous definition of $\chi_{j_Ej_E}(\omega)$. For further discussion it is convenient to present and analyze also corresponding memory functions $M(\omega)$ and $N(\omega)$ defined, respectively, as[17]

$$\sigma(\omega)=\frac{i}{L}\frac{\chi^0_{jj}}{\omega+M(\omega)},\quad \kappa(\omega)=\frac{i\beta}{L}\frac{\chi^0_{j_Ej_E}}{\omega+N(\omega)}. \tag{7}$$

Note that finite coherent component D represents the strength of the $\delta(\omega)$ contribution in $\sigma'(\omega)$ requiring $\chi_{jj}(\omega\to 0)<\chi^0_{jj}$ or from Eq. (7) $M''(\omega=0)=0$. On the other hand, any finite $M''(\omega)>0$ means the finite decay rate of the spin current as well as a finite dc conductivity $\sigma_0=\sigma(\omega=0)<\infty$, i.e., strictly $D=0$.

We use further the advantage of studying closer $\kappa(\omega)$ (instead of $\sigma(\omega)$) since j_E is a conserved quantity in the pure AHM,[6] hence $N_0(\omega)=0$ and consequently $N(\omega)\neq 0$ appears only due to $b_0\neq 0$. On the other hand, j is not conserved and $M(\omega)=M_0(\omega)$ is nontrivial even in the absence of impurities. Nevertheless, $M''_0(\omega=0)=0$ at any T as required to obtain $D(T)>0$. In the following we evaluate $\sigma(\omega)$ and $\kappa(\omega)$ at $T>0$ using the microcanonical Lanczos method (MCLM) (Ref. 18) to calculate the dynamical susceptibilities in systems with $L=16-24$. Typically, $N_L\sim 2000$ Lanczos steps are used to obtain spectra with high ω resolution, so that the additional broadening is only $\delta=0.01$. In the following we present merely results at $\beta\to 0$, which do not qualitatively change with T down to $T\sim J$. At least for larger L smooth $\sigma(\omega)$ and $\kappa(\omega)$ then allow the evaluation of $M(\omega)$ and $N(\omega)$ via Eq. (7).

Let us start with the analysis of (real part) $\kappa'(\omega)$, which reveals a Lorentzian (Drude) form for $\Delta=0.5, b_0=0.5$ as shown in Fig. 4(a). Moreover, results show universal size scaling as $\kappa'(L\omega)/L$. Hence, corresponding $N''(\omega)$ also scales as $1/L$, so that the size-independent quantity is $\tilde{N}(\omega)=LN(\omega)$ being quite structureless for $\omega<1$ as shown in Fig. 4(b). It is also evident from Fig. 4(c) that $N''(\omega)\propto b_0^2$ at least for weaker $b_0<0.5$. On the other hand, at larger $b_0>0.5 N''(\omega)$ obtains a characteristic peak at low $\omega\to 0$ which strongly reduces the dc value $\kappa(\omega=0)$. I.e., on entering the regime $b_0>1$ the impurity starts to cut the ring for the dc transport.

The regular behavior of $N''(\omega)$ for weaker $b_0<1$ gives support to the attempt to evaluate the memory function within the perturbation approach[17] using the force-force correlations,

$$N_p(\omega)=\frac{1}{\omega\chi^0_{j_Ej_E}}(\chi_{ff}(\omega)-\chi^0_{ff}),\quad f=i[H,j_E], \tag{8}$$

where $\chi_{ff}(\omega)$ is the force-force dynamical susceptibility. Results for $N''_p(\omega)/L$ evaluated using eigenstates obtained by the ED of the system $L=14$ are for comparison also presented in Fig. 4(b). The correspondence is quite satisfactory.

Finally, we present in Fig. 5 also analogous scaled σ'/L vs $L\omega$ and corresponding $M''(\omega)$ for fixed $\Delta=0.5, b_0=0.6$ and different $L=16-24$, as obtained via the ED ($L=16$) and

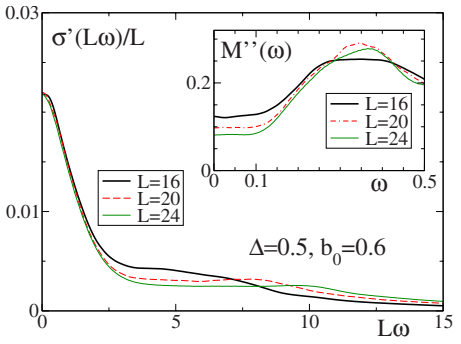

FIG. 5. (Color online) (a) Scaled spin conductivity σ'/L vs $L\omega$ for different $L=16-24$, and (b) corresponding $M''(\omega)$.

MCLM ($L=20,24$) at $\beta\to 0$. Since $M_0(\omega)$ is nontrivial even for $b_0=0$ one can discuss possible decomposition $M(\omega)=M_0(\omega)+\tilde{M}(\omega)/L$. Results confirm that at low $\omega<0.2$ $\sigma(\omega)$ reveals a Lorentzian with $M''(\omega\to 0)$ scaling as $1/L$, the only contribution in this regime coming from the impurity.

It should be pointed out that obtained incoherent transport is characterized with the relaxation times τ and dc conductivities scaling linearly with L, as expected for 1D systems with a single perturbed region. Hence, the length independent quantities are $\sigma(0)/L=\chi^0_{jj}/[LM''(\omega=0)]=\chi^0_{jj}/\tilde{M}''(\omega=0)$ and the corresponding thermal one $\kappa(0)/L=\beta\chi^0_{j_E j_E}/\tilde{N}''(\omega=0)$.

In conclusion, we have shown that the transport in the considered anisotropic Heisenberg model on the ring with a single static impurity is quite unique. Since both the spin (for $\Delta<1$) and thermal conductivity at any $T>0$ are dissipationless in the pure system, one can study directly the nontrivial effect of a single impurity on the level statistics and transport in the many-body quantum system. We have shown that single static impurity induces an incoherent transport with a well-defined current relaxation time which scales as $\tau\propto L$. This should be contrasted with the case of noninteracting fermions in Eq. (5) where a single impurity only reduces the stiffness D but does not lead to the current relaxation within the ring at any T. The fundamental difference seems to come from the umklapp processes which are revived by the impurity and lead to the decoherence between successive scattering events on the impurity. In this sense it is also plausible that for a finite but low concentration c_i of static impurities in a chain (as relevant for experiments)[12] we expect that our results can be simply generalized as $1/\tau\propto 1/L\to c_i$, as evident also from the lowest-order perturbation theory, Eq. (8).

Although we studied here the AHM model, results, and conclusions could be plausibly generalized to 1D integrable chain systems with periodic boundary conditions and a localized perturbed region. In this paper we presented only results in the high-T regime, still the phenomenon is expected to persist as far as the umklapp processes are effective, i.e., for T above some characteristic umklapp temperature T_U. We can speculate that the LL phenomenology[1,2] can become effective only for $T\ll T_U$, whereby there is another Kane-Fisher scale T^* which divides the regimes of cut chain for $T<T^*$ and renormalized coherent transmission for $T>T^*$. Further studies are needed to establish these scales for relevant impurities and models. In any case, such phenomena are expected to be relevant in connection with recent experiments on thermal conductivity in spin chains with dilute impurities.[12]

This work was supported by the FP6-032980-2 NOVMAG and COST P-16 ECOM project and by the Slovenian Agency under Grant No. P1-0044.

[1] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992); Phys. Rev. B **46**, 15233 (1992).
[2] A. Furusaki and N. Nagaosa, Phys. Rev. B **47**, 4631 (1993).
[3] V. Meden and U. Schollwöck, Phys. Rev. B **67**, 035106 (2003).
[4] S. Rommer and S. Eggert, Phys. Rev. B **62**, 4370 (2000).
[5] H. Castella, X. Zotos, and P. Prelovšek, Phys. Rev. Lett. **74**, 972 (1995).
[6] X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B **55**, 11029 (1997).
[7] For a review see T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. M. Wong, Rev. Mod. Phys. **53**, 385 (1981).
[8] Ph. Jacquod and D. L. Shepelyansky, Phys. Rev. Lett. **79**, 1837 (1997); B. Georgeot and D. L. Shepelyansky, *ibid.* **81**, 5129 (1998).
[9] D. A. Rabson, B. N. Narozhny, and A. J. Millis, Phys. Rev. B **69**, 054403 (2004).
[10] A. Karahalios, A. Metavitsiadis, X. Zotos, A. Gorczyca, and P. Prelovšek, Phys. Rev. B **79**, 024425 (2009).
[11] P. Schmitteckert, T. Schulze, C. Schuster, P. Schwab, and U. Eckern, Phys. Rev. Lett. **80**, 560 (1998).
[12] For a review see C. Hess, Eur. Phys. J. Spec. Top. **151**, 73 (2007).
[13] L. F. Santos, J. Phys. A **37**, 4723 (2004).
[14] D. Mulhall, Z. Huard, and V. Zelevinsky, Phys. Rev. C **76**, 064611 (2007).
[15] M. Di Stasio and X. Zotos, Phys. Rev. Lett. **74**, 2050 (1995).
[16] T. Rejec and A. Ramšak, Phys. Rev. B **68**, 033306 (2003).
[17] W. Götze and P. Wölfle, Phys. Rev. B **6**, 1226 (1972).
[18] M. W. Long, P. Prelovšek, S. El Shawish, J. Karadamoglou, and X. Zotos, Phys. Rev. B **68**, 235106 (2003).