

This is the accepted manuscript made available via CHORUS. The article has been published as:

Exact results for nonlinear Drude weights in the spin- $\frac{1}{2}$ XXZ chain

Yuhi Tanikawa, Kazuaki Takasan, and Hosho Katsura

Phys. Rev. B **103**, L201120 — Published 27 May 2021

DOI: [10.1103/PhysRevB.103.L201120](https://doi.org/10.1103/PhysRevB.103.L201120)

Exact results for nonlinear Drude weights in the spin-1/2 XXZ chain

Yuhi Tanikawa,¹ Kazuaki Takasan,² and Hosho Katsura^{1,3,4}

¹*Department of Physics, The University of Tokyo,
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*

²*Department of Physics, University of California, Berkeley, California 94720, USA*

³*Institute for Physics of Intelligence, The University of Tokyo,
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*

⁴*Trans-scale Quantum Science Institute, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan*

(Dated: May 12, 2021)

Nonlinear Drude weight (NLDW) is a generalization of the linear Drude weight, which characterizes the nonlinear transport in quantum many-body systems. We investigate these weights for the spin-1/2 XXZ chain in the critical regime. The effects of the Dzyaloshinskii-Moriya interaction and an external magnetic field are also studied. Solving the Bethe equations numerically, we obtain these weights for very large system sizes and identify parameter regimes where the weights diverge in the thermodynamic limit. These divergences appear in all the orders studied in this paper and can be regarded as a generic feature of the NLDWs. We study the origin of these divergences and reveal that they result from *nonanalytic* finite-size corrections to the ground state energy. Furthermore, we compute closed-form expressions for several weights in the thermodynamic limit and find excellent agreement with the numerical results.

Introduction. — Transport phenomena have been one of the most important subjects in condensed matter and statistical physics. The linear transport phenomena are well explained by the famous linear response theory [1] and widely applied to many experiments. On the other hand, the nonlinear responses are less understood [2] and we still do not have a systematic understanding of them. While the nonlinear responses have been well-studied in the field of nonlinear optics [3, 4], they are still an intriguing topic. For instance, rectification currents [5, 6] and high-harmonic generations [7, 8] in solids are experimentally observed and extensively studied recently. They are used as new experimental probes and expected to be utilized for future optical/electric devices. Stimulated by this situation, the theoretical investigation for nonlinear responses is rapidly developing [9–15], but further studies are still desired. In particular, the understanding of the nonlinear responses in many-body interacting systems is still poor compared with the non-interacting case [16–18].

Very recently, *nonlinear Drude weights* (NLDWs) characterizing the nonlinear static transport have been introduced [19, 20]. This is an extension of the linear Drude weight which was introduced by Kohn as an indicator to distinguish metals and insulators in quantum many-body systems [21] and has been extensively studied in various contexts related to transport phenomena. In particular, the Drude weight is calculable with the exact solutions of one-dimensional quantum many-body systems and thus has been a principal quantity in the studies of their transport phenomena at zero and finite temperature [22]. As the linear one has played a very important role, the NLDWs are also expected to provide useful information about nonlinear transport even in interacting many-body systems. However, most of the properties of NLDWs are still unexplored. For example, Ref. [19] reported the divergent behavior of the third-order Drude weight in the spin-1/2 XXZ chain. This is

regarded as a feature of NLDWs not existing in linear Drude weights, and calls for a more detailed analysis of NLDWs, especially in interacting systems.

In this paper, we study the NLDWs at zero temperature in the spin-1/2 XXZ chain, which is a prototypical many-body interacting model [23]. The linear Drude weight of this model has been extensively studied in quantum transport phenomena [22, 24–29]. The most important advantage of this model is its solvability by the Bethe ansatz [30, 31], which enables us to treat very large system sizes. We also study the effect of the Dzyaloshinskii-Moriya (DM) interaction with a uniform DM vector along the z axis [32] and an external magnetic field which are treatable within the Bethe ansatz technique. By using the exact solutions, we calculate the first several orders of the NLDWs numerically and find parameter regimes where the weights diverge in the thermodynamic limit. While this divergence never appears in the linear one, it appears in all the NLDWs studied in this paper. Thus, we consider that the divergent behavior is one of the generic features of the NLDWs in interacting systems. To clarify the origin of this divergence, we analyze the finite size corrections to the ground state energy of the model. The detailed analysis shows that the divergence comes from a nonanalytic term proportional to a noninteger power of $1/N$ (N : system size). We explicitly identify the noninteger powers and confirmed the expected divergence by using our numerical results. Furthermore, we derive closed-form expressions in the thermodynamic limit for several NLDWs in the convergent region by using the Wiener-Hopf method [30, 33–35]. The obtained results match the numerical results with high accuracy.

Models. — The spin-1/2 XXZ chain is defined by the

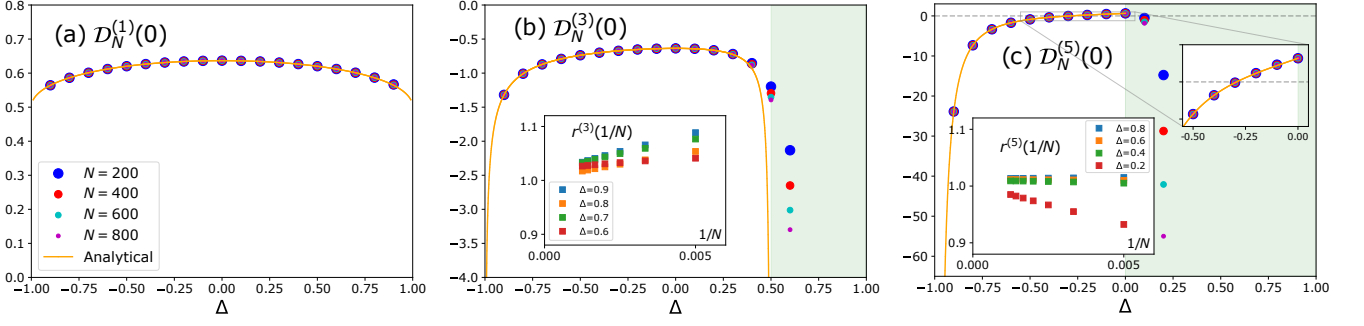


FIG. 1. Numerical and analytical results for $\mathcal{D}_N^{(n)}(0)$ ($n = 1, 3, 5$). All the vertical axes are scaled with J . NLDWs $\mathcal{D}_N^{(3)}(\Theta)$ and $\mathcal{D}_N^{(5)}(\Theta)$ diverge in green regions, which are determined by $4\gamma/(\pi - \gamma) < n - 1$. The insets in (b) and (c) show $r^{(n)}(1/N)$ [Eq. (11)] in the divergent regions and confirm the divergence caused by *noninteger* powers of $1/N$.

Hamiltonian:

$$\hat{\mathcal{H}}(0) = \sum_{l=1}^N 2J \left[\hat{S}_l^x \hat{S}_{l+1}^x + \hat{S}_l^y \hat{S}_{l+1}^y + \Delta \hat{S}_l^z \hat{S}_{l+1}^z \right], \quad (1)$$

where $\hat{S}_l^\alpha$ ($\alpha = x, y, z$) are spin-1/2 operators, $J > 0$ is the coupling constant, Δ is the anisotropy parameter, and N is the number of sites. We assume that $-1 < \Delta < 1$ and N is even throughout this paper. Note that this model is mapped to the interacting spinless fermion model via the Jordan-Wigner transformation [30]. In this model, the Hamiltonian with the $U(1)$ flux Φ reads

$$\hat{\mathcal{H}}(\Phi) = \sum_{l=1}^N 2J \left[\frac{1}{2} e^{i\frac{\Phi}{N}} \hat{S}_l^+ \hat{S}_{l+1}^- + \text{h.c.} + \Delta \hat{S}_l^z \hat{S}_{l+1}^z \right], \quad (2)$$

where $\hat{S}_l^\pm = \hat{S}_l^x \pm i\hat{S}_l^y$. Here it is enough to consider only $-\pi < \Phi \leq \pi$, as $\mathcal{H}(\Phi)$ and $\mathcal{H}(\Phi + 2\pi)$ have the same spectrum. The $\Phi \neq 0$ case corresponds to the spin-1/2 XXZ chain with the DM interaction [32, 36]. When we consider the effect of an external magnetic field, we add to the Hamiltonian the term $-h \sum_{l=1}^N \hat{S}_l^z$ where h is the magnetic field.

Since the total magnetization $\hat{S}_{\text{tot}}^z = \sum_{l=1}^N \hat{S}_l^z$ is conserved even under the magnetic field, we can obtain the lowest energy state in each sector individually by the Bethe ansatz [37]. In the sector with M down spins, the Bethe roots $\{v_j(\Phi)\}$ are determined by the following Bethe equation for $j = 1, 2, \dots, M$:

$$p_1(v_j(\Phi)) + \frac{\Phi}{N} - \frac{1}{N} \sum_{k=1}^M p_2(v - v_k(\Phi)) = \frac{\pi}{N} (-M + 2j - 1), \quad (3)$$

where $p_n(v) \equiv 2 \tan^{-1} \left(\frac{\tanh \frac{\gamma}{2} v}{\tan \frac{\gamma}{2}} \right)$ and $\gamma \equiv \arccos \Delta$. Us-

ing the Bethe roots, the energy density is given as

$$e(\Phi, h; M) = \frac{1}{N} \sum_{j=1}^M \frac{2J \sin^2 \gamma}{\cos \gamma - \cosh \gamma v_j(\Phi)} + \frac{J\Delta}{2} - h \left(\frac{1}{2} - \frac{M}{N} \right). \quad (4)$$

If $h = 0$ and $\Phi = 0$, it is known that the ground state lies in the sector of $M = N/2$ [38]. Thus, for sufficiently small Φ the ground state energy density of $\mathcal{H}(\Phi)$ is $e_{\text{gs}}(\Phi) = e(\Phi, h = 0; M = N/2)$ [39]. Under the magnetic field h , M is not necessarily equal to $N/2$ and the ground state energy density is given as $e_{\text{gs}}(\Phi, h) = \min_M e(\Phi, h; M)$.

Nonlinear Drude weight. — Let us introduce the NLDWs. We follow the argument of Ref. [19]. We consider the application of the time-dependent flux $\Phi(t) \equiv N\phi(t)$. This induces the spin current density $j_s(t) = \langle \psi(t) | \partial \hat{\mathcal{H}}(\Phi) / \partial \Phi | \psi(t) \rangle$. Here, the state at time t is defined as $|\psi(t)\rangle = U(t) |\psi_0\rangle$ where $\hat{U}(t) = \mathcal{T} \exp[-i \int_0^t \hat{\mathcal{H}}(\Phi(s)) ds]$ is the time-evolution operator and $|\psi_0\rangle$ is the ground state of $\hat{\mathcal{H}}(\Phi(0))$. Then, we define the linear and nonlinear conductivities in real time as

$$j_s(t) - j_s(0) = \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 \cdots \int_0^t dt_n \times \sigma^{(n)}(t - t_1, \dots, t - t_n) \prod_{l=1}^n \left(-\frac{d\phi(t_l)}{dt_l} \right). \quad (5)$$

Since the response function $\sigma^{(n)}(t_1, \dots, t_n)$ vanishes whenever $t_l < 0$ for any $l = 1, 2, \dots, n$ due to the causality, the Fourier transform is given as $\sigma^{(n)}(\omega_1, \dots, \omega_n) = \int_0^\infty dt_1 \cdots \int_0^\infty dt_n \sigma^{(n)}(t_1, \dots, t_n) \prod_{l=1}^n e^{i(\omega_l + i0)t_l}$. The n -th order Drude weights in a finite system $\mathcal{D}_N^{(n)}$ are defined by the most singular part of $\sigma^{(n)}(\omega_1, \dots, \omega_n)$ around $\omega_1, \dots, \omega_n = 0$ and thus reads

$$\sigma_{\text{Drude}}^{(n)}(\omega_1, \dots, \omega_n) = \mathcal{D}_N^{(n)} \prod_{l=1}^n \frac{i}{\omega_l + i0}, \quad (6)$$

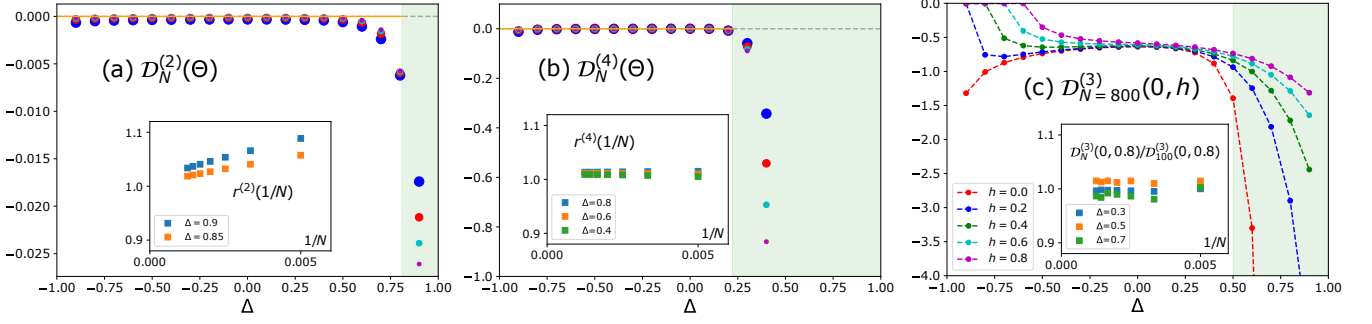


FIG. 2. Numerical and analytical results for $\mathcal{D}_N^{(n)}(\Theta = 0.1)$ ($n = 2, 4$) are shown in (a) and (b). Symbols are the same as in Fig. (1). Numerical results for $\mathcal{D}_{N=800}^{(3)}(0, h)$ are shown in (c). All the vertical axes are scaled with J . Green regions are the divergent regions of NLDWs without a magnetic field, which are determined by $4\gamma/(\pi - \gamma) < n - 1$. The insets in (a) and (b) show $r^{(n)}(1/N)$ [Eq. (11)] in the divergent regions and confirm the divergence caused by *noninteger* powers of $1/N$. The inset in (c) shows $\mathcal{D}_N^{(3)}(0, h = 0.8)/\mathcal{D}_{100}^{(3)}(0, h = 0.8)$ and confirms the convergence.

where the n -th order conductivity is decomposed as $\sigma^{(n)} = \sigma_{\text{Drude}}^{(n)} + \sigma_{\text{regular}}^{(n)}$ [23]. At zero temperature, NLDWs $\mathcal{D}_N^{(n)}$ can be calculated as

$$\mathcal{D}_N^{(n)}(\Theta) = N^{n+1} \frac{\partial^{n+1}}{\partial \Phi^{n+1}} e_{\text{gs}}(\Phi) \Big|_{\Phi=\Theta}. \quad (7)$$

This is the one-dimensional version of the nonlinear Kohn formula derived in Refs. [19] and [20] which provide two different derivations, respectively. The finite Θ corresponds to the DM interaction as mentioned above. Under a finite magnetic field, we define $\mathcal{D}_N^{(n)}(\Theta, h)$ with replacing $e_{\text{gs}}(\Phi)$ by $e_{\text{gs}}(\Phi, h)$ in Eq. (7). Note that the spin current corresponds to the electric (particle) current when the spin chain is mapped to the fermionic chain and thus the NLDWs defined above are related not only to the spin transport but also to more generic transport properties in interacting many-body systems.

Numerical results. — By numerically solving the Bethe equations [Eq. (3)], we calculate the NLDWs $\mathcal{D}_N^{(n)}(\Theta)$. To calculate them, we approximate the derivative in Eq. (7) by finite differences.

First, we study the $\Theta = 0$ case where only the odd orders are nonvanishing. This is because the ground state energy density $e_{\text{gs}}(\Phi)$ is an even function of Φ [40]. It corresponds to the fact that the even order nonlinear responses vanish in inversion symmetric systems, which is well-known in nonlinear optics [3, 4]. The results for $\mathcal{D}_N^{(n)}(0)$ ($n = 1, 3, 5$) are shown in Figs. 1 (a)-(c). Fig. 1 (a) is consistent with the previous work [24], and Fig. 1 (b) is also consistent with the recent numerical results for small system sizes [19]. The most significant difference between the linear and nonlinear ones is the existence of divergent regions. The third-order one $\mathcal{D}_N^{(3)}(0)$ and the fifth-order one $\mathcal{D}_N^{(5)}(0)$ tend to diverge for $0.5 \lesssim \Delta < 1$ and $0 \lesssim \Delta < 1$, respectively. Note that $\mathcal{D}_N^{(5)}(0)$ crosses zero at $\Delta \simeq -0.29$ and changes its sign when passing through the point as seen in Fig. 1 (c). This is a unique feature which does not appear in the lower

orders and there might arise some special properties at this point. We also note in passing that a divergent behavior similar to that of $\mathcal{D}_N^{(3)}(0)$ was found for the fourth derivative of the ground state energy density with respect to the magnetization [41].

Next, we consider the $\Theta \neq 0$ case. As we mentioned, this corresponds to the XXZ spin chain with finite DM interaction which breaks the inversion symmetry. Thus, even order responses are allowed. The results for $\mathcal{D}_N^{(n)}(\Theta \neq 0)$ ($n = 2, 4$) are shown in Figs. 2 (a) and (b). As we expected, $\mathcal{D}_N^{(n)}(\Theta \neq 0)$ is nonzero in finite systems. We can see the convergence of $\mathcal{D}_N^{(n)}(\Theta \neq 0)$ ($n = 2, 4$) to 0 in a wide range of Δ in the thermodynamic limit. The interesting point is that there also exist the divergent regions, as seen in Figs. 1 (b) and (c). The second-order one $\mathcal{D}_N^{(2)}(\Theta \neq 0)$ and the fourth-order one $\mathcal{D}_N^{(4)}(\Theta \neq 0)$ tend to diverge for $0.81 \lesssim \Delta < 1$ and $0.22 \lesssim \Delta < 1$, respectively. Since the effect of the flux Θ is rewritten as a twisted boundary condition, the ground state energy density is expected to be independent of Θ in the thermodynamic limit. Thus, it might seem that $\mathcal{D}_N^{(n)}(\Theta \neq 0)$ is zero. However, since the Drude weights are differential coefficients before taking the thermodynamic limit, the divergence does not contradict the above statement. This reflects that the thermodynamic limit and the differentiation with respect to Φ are not interchangeable.

Finally, we study the effect of the magnetic field. The results for $\mathcal{D}_{N=800}^{(3)}(0, h)$ are shown in Fig. 2 (c). For the Δ around both -1 and 1 , the values are suppressed. Some of the values around $\Delta = -1$ reach zero. It is natural because the gapped regime comes into $|\Delta| < 1$ under the magnetic field [30]. The more nontrivial one is around $\Delta = 1$. It seems that the divergent behavior is suppressed by the magnetic field. Indeed, the N dependence shown in the insets of Fig. 2 (c) confirms that the convergent region becomes wider under the magnetic field. As we discuss later, this behavior can be understood from the low-energy effective field theory. Note

that these properties are seen in other orders of NLDWs as well [42].

Origin and properties of the divergence. — As Figs. 1 and 2 imply, the NLDWs diverge in the certain regions by taking the thermodynamic limit. While the same behavior in the third-order one was reported based on numerical diagonalization [19], the origin remains unclear. Here, we show that these behaviors are caused by the special terms included in the power series expansion of $e_{\text{gs}}(\Phi)$. The finite size corrections to the ground-state energy of the XXZ spin chain have been studied in great detail [43–48]. Previous studies revealed that the corrections include both integer and noninteger powers of $1/N$, both of which can be accounted for by considering the low-energy effective field theory of the XXZ chain, i.e., the $c = 1$ conformal field theory (CFT) perturbed by irrelevant operators. Although the effect of the flux has not been fully explored, it is natural to assume that the coefficient of each correction term can be Taylor expanded around $\Phi = 0$. This, together with the fact that $e_{\text{gs}}(\Phi)$ is an even function of Φ , yields

$$e_{\text{gs}}(\Phi) - e_{\text{gs}}(0) = \sum_{k \geq l \geq 1} A_{k,l} \left(\frac{1}{N}\right)^{2k} \Phi^{2l} + \sum_{k,l,m \geq 1} B_{k,l,m} \left(\frac{1}{N}\right)^{2k+4m\frac{\gamma}{\pi-\gamma}} \Phi^{2l}, \quad (8)$$

where $A_{k,l}$ and $B_{k,l,m}$ are coefficients depending on the parameter γ . Note that the coefficients $A_{1,1}$, $A_{2,2}$, and $B_{1,1,1}$ can be read off from Eq. (4.1) in Ref. [48], and at the free-fermion point ($\gamma = \pi/2$), all the coefficients can be easily computed explicitly [19]. In the following, for simplicity, we restrict ourselves to the case where γ is generic, i.e., none of the exponents in the second sum are integers. The noninteger exponent can be rewritten as $2k + 4m\gamma/(\pi - \gamma) = 2k + 4m(2K - 1)$, where $K = (\pi/2)/(\pi - \gamma)$ is the Tomonaga-Luttinger parameter of the model [34, 49, 50]. This reflects that the nonanalytic finite size corrections originate from irrelevant operators with noninteger scaling dimensions such as $4K$ [45, 46].

Any term Φ^α/N^β ($\alpha > \beta$) in Eq. (8) can contribute to divergences of NLDWs. The straightforward calculation gives

$$\mathcal{D}_N^{(2k-1)}(\Theta) = (2k)! \left[A_{k,k} + B_{1,k,1} N^{2k-2-\frac{4\gamma}{\pi-\gamma}} + \dots \right], \quad (9)$$

$$\mathcal{D}_N^{(2k)}(\Theta) = (2k+2)! A_{k+1,k+1} \frac{\Theta}{N} + C_k(\Theta) N^{2k-1-\frac{4\gamma}{\pi-\gamma}} + \dots, \quad (10)$$

where $C_k(\Theta) \equiv \sum_{l > k} (2l)!/(2l - 2k - 1)! B_{1,l,1} \Theta^{2l-2k-1}$. The above expressions suggest that $\mathcal{D}_N^{(2k-1)}(\Theta)$ and $\mathcal{D}_N^{(2k)}(\Theta)$ are likely to diverge when the exponent of the power of N in each second term, which can be the leading term, is positive: $2k > 2 + 4\gamma/(\pi - \gamma)$ and

$2k > 1 + 4\gamma/(\pi - \gamma)$, respectively [51]. This enabled us to determine the green regions in Figs. 1 and 2.

Also, Eqs. (9) and (10) imply that $\mathcal{D}_N^{(n)}(\Theta)$ shows the divergence caused by $N^{n-1-\frac{4\gamma}{\pi-\gamma}}$ in the divergent region. In order to confirm this, we define $r^{(2k-1)}(1/N)$ and $r^{(2k)}(1/N)$ as

$$r^{(2k-1)}(1/N) = \frac{\mathcal{D}_N^{(2k-1)}(0)}{(2k)! B_{1,k,1} N^{2k-2-4\gamma/(\pi-\gamma)}}, \quad (11)$$

$$r^{(2k)}(1/N) = \frac{\mathcal{D}_N^{(2k)}(\Theta)}{C_k(\Theta) N^{2k-1-4\gamma/(\pi-\gamma)}}, \quad (12)$$

and plot Eq. (11) [Eq. (12)] in the insets of Figs. 1 (b) and (c) [Figs. 2 (a) and (b)]. These figures clearly show that each data is on a straight line to the value near 1 in the large N region, indicating that the divergences are caused by the *noninteger* power terms of N expected from the power series expansion (8). We stress that the numerical confirmation of these behaviors is quite challenging because it requires large system sizes, which are beyond the reach of other numerical methods such as exact diagonalization.

The suppression of the divergence under the magnetic field around $\Delta = 1$, shown in Fig. 2 (c), is also explained by the expansion (8). In the absence of the magnetic field, the umklapp scattering term with scaling dimension $4K = 2\pi/(\pi - \gamma)$ is responsible for the nonanalytic finite-size corrections. However, in the presence of the magnetic field, the Fermi wave vectors become incommensurate with the lattice. As a result, the umklapp term oscillates in space and should be dropped in a renormalization group sense [34, 49, 52]. Therefore, the effect of noninteger powers in Eq. (8) are expected to be small under the magnetic field and thus the divergence is suppressed as well.

Analytical form in the convergent region. — By using the expansion [Eq. (8)], we can derive closed-form expressions for NLDWs in the thermodynamic limit. Taking the limit in Eq. (8) in the convergent region, we obtain the NLDWs $\mathcal{D}^{(2k)} = 0$ and $\mathcal{D}^{(2k-1)} = (2k)! A_{k,k}$ where $\mathcal{D}^{(n)} \equiv \lim_{N \rightarrow \infty} \mathcal{D}_N^{(n)}(\Theta)$, and thus the problem is reduced to the calculation of $A_{k,k}$. These coefficients can be calculated using the Wiener-Hopf method, which is a mathematical technique to solve the Wiener-Hopf integral equations [30, 33–35] (see Supplemental Material for more details). As a result, the first-order (linear) one is

$$\mathcal{D}^{(1)} = \frac{\pi J \sin \gamma}{2\gamma(\pi - \gamma)}, \quad (13)$$

for $0 < \gamma < \pi$. This is consistent with the previous works [24, 25]. The third-order and fifth-order ones are given by

$$\mathcal{D}^{(3)} = -\frac{J \sin \gamma}{8\gamma(\pi - \gamma)} \left[\frac{\Gamma(\frac{3\pi}{2\gamma}) \Gamma(\frac{\pi-\gamma}{2\gamma})^3}{\Gamma(\frac{3(\pi-\gamma)}{2\gamma}) \Gamma(\frac{\pi}{2\gamma})^3} + \frac{3\pi \tan(\frac{\pi^2}{2\gamma})}{\pi - \gamma} \right], \quad (14)$$

for $\pi/3 < \gamma < \pi$, and

$$\mathcal{D}^{(5)} = \frac{3J \sin \gamma}{32\pi\gamma(\pi - \gamma)} \left[\frac{\Gamma(\frac{5\pi}{2\gamma})\Gamma(\frac{\pi-\gamma}{2\gamma})^5}{\Gamma(\frac{5(\pi-\gamma)}{2\gamma})\Gamma(\frac{\pi}{2\gamma})^5} - \frac{5}{3} \cdot \frac{\Gamma(\frac{3\pi}{2\gamma})^2\Gamma(\frac{\pi-\gamma}{2\gamma})^6}{\Gamma(\frac{3(\pi-\gamma)}{2\gamma})^2\Gamma(\frac{\pi}{2\gamma})^6} + \frac{15\pi^2 \tan^2(\frac{\pi}{2\gamma})}{(\pi - \gamma)^2} + \frac{5\pi \tan(\frac{\pi}{2\gamma})}{\pi - \gamma} \cdot \frac{\Gamma(\frac{3\pi}{2\gamma})\Gamma(\frac{\pi-\gamma}{2\gamma})^3}{\Gamma(\frac{3(\pi-\gamma)}{2\gamma})\Gamma(\frac{\pi}{2\gamma})^3} \right], \quad (15)$$

for $\pi/2 < \gamma < \pi$, respectively. We note that the result of $\mathcal{D}^{(3)}$ can also be read off from $A_{2,2}$ in Eq. (8) and is consistent with the result of Ref. [19]. These are plotted in Fig. 1. Clearly, the analytical results match the numerical results with high accuracy.

Conclusion and Outlook. — In this study, we calculated the zero-temperature NLDWs of the spin-1/2 XXZ chain in the critical regime numerically for large system sizes, considering the effect of the DM interaction or the external magnetic field. The numerical results [Figs. 1 and 2] revealed that all the NLDWs diverge in certain Δ regions by taking the thermodynamic limit. Thus, we considered these divergences are a generic feature in interacting systems and investigated their mechanism. Based on the power series expansion [Eq. (8)], we identified the origin of the divergences as nonanalytic finite-size corrections to the ground state energy. This expansion also allows us to identify the regions and strength of the divergences. We confirmed that they are in good agreement with the

numerical data. Furthermore by using the Wiener-Hopf method, we obtained the closed forms of several weights in the thermodynamic limit [Eqs. (13)-(15)]. In the convergent regions, they matched the numerical results with high accuracy as seen in Fig. 1. Although in this paper we calculated the analytical expressions for NLDWs by treating the magnetization and the U(1) flux simultaneously (see Supplemental Material), we expect that a direct calculation for zero magnetization should be possible using another method involving nonlinear integral equations [53]. A thorough analysis of NLDWs based on such a sophisticated method would be an interesting future direction.

Our results are a first systematic calculation of the NLDWs in interacting many-body systems for very large system sizes. We found that the divergent behavior generically appears and clarified the origin of the divergence. We believe that our results will help understanding the nonlinear transport in quantum many-body systems.

ACKNOWLEDGMENTS

We thank Haruki Watanabe, Masaki Oshikawa, and Kiyohide Nomura for valuable discussions. K. T. thanks JSPS for support from Overseas Research Fellowship. H. K. was supported in part by JSPS Grant-in-Aid for Scientific Research on Innovative Areas No. JP20H04630, JSPS KAKENHI Grant No. JP18K03445, and the Inamori Foundation.

-
- [1] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
 - [2] A. Shimizu, J. Phys. Soc. Jpn. **79**, 113001 (2010).
 - [3] R. W. Boyd, *Nonlinear Optics, Third Edition*, 3rd ed. (Academic Press, London, 2008).
 - [4] N. Bloembergen, *Nonlinear Optics*, 4th ed. (World Scientific, Singapore, 1996).
 - [5] L. Z. Tan, F. Zheng, S. M. Young, F. Wang, S. Liu, and A. M. Rappe, npj Comp. Mat. **2**, 16026 (2016).
 - [6] Y. Tokura and N. Nagaosa, Nat. Comm. **9**, 3740 (2018).
 - [7] S. Y. Kruchinin, F. Krausz, and V. S. Yakovlev, Rev. Mod. Phys. **90**, 021002 (2018).
 - [8] S. Ghimire and D. A. Reis, Nat. Phys. **15**, 10 (2019).
 - [9] I. Sodemann and L. Fu, Phys. Rev. Lett. **115**, 216806 (2015).
 - [10] T. Morimoto and N. Nagaosa, Sci. Adv. **2** (2016), 10.1126/sciadv.1501524.
 - [11] F. de Juan, A. G. Grushin, T. Morimoto, and J. E. Moore, Nat. Comm. **8**, 15995 (2017).
 - [12] D. E. Parker, T. Morimoto, J. Orenstein, and J. E. Moore, Phys. Rev. B **99**, 045121 (2019).
 - [13] H. Isobe, S.-Y. Xu, and L. Fu, Sci. Adv. **6** (2020), 10.1126/sciadv.aay2497.
 - [14] J. Ahn, G.-Y. Guo, and N. Nagaosa, Phys. Rev. X **10**, 041041 (2020).
 - [15] K. Takasan, T. Morimoto, J. Orenstein, and J. E. Moore, “Current-induced second harmonic generation in inversion-symmetric dirac and weyl semimetals,” (2020), arXiv:2007.08887 [cond-mat.mes-hall].
 - [16] T. Morimoto and N. Nagaosa, Sci. Rep. **8**, 2973 (2018).
 - [17] A. Avdoshkin, V. Kozii, and J. E. Moore, Phys. Rev. Lett. **124**, 196603 (2020).
 - [18] Y. Michishita and R. Peters, “Correlation effect on nonlinear responses in strongly-correlated electron systems,” (2021), arXiv:2012.10603 [cond-mat.str-el].
 - [19] H. Watanabe and M. Oshikawa, Phys. Rev. B **102**, 165137 (2020).
 - [20] H. Watanabe, Y. Liu, and M. Oshikawa, J. Stat. Phys. **181**, 2050 (2020).
 - [21] W. Kohn, Phys. Rev. **133**, A171 (1964).
 - [22] B. Bertini, F. Heidrich-Meisner, C. Karrasch, T. Prosen, R. Steinigeweg, and M. Znidaric, (2020), arXiv:2003.03334.
 - [23] The Drude weights in this paper are often called *spin* Drude weight since this is related to the spin current [22].
 - [24] B. Sutherland and B. S. Shastry, Phys. Rev. Lett. **65**, 1833 (1990).
 - [25] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
 - [26] V. Korepin and A. Wu, Int. J. Mod. Phys. B **05**, 497 (1991), <https://doi.org/10.1142/S0217979291000304>.

- [27] B. N. Narozhny, A. J. Millis, and N. Andrei, Phys. Rev. B **58**, R2921 (1998).
- [28] X. Zotos, Phys. Rev. Lett. **82**, 1764 (1999).
- [29] J. Benz, T. Fukui, A. Klümper, and C. Scheeren, J. Phys. Soc. Jpn. **74**, 181 (2005), <https://doi.org/10.1143/JPSJS.74S.181>.
- [30] M. Takahashi, *Thermodynamics of one-dimensional solvable models* (Cambridge university press, 2005).
- [31] V. E. Korepin, N. M. Bogoliubov, and A. G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions*, Cambridge Monographs on Mathematical Physics (Cambridge University Press, 1993).
- [32] F. C. Alcaraz and W. F. Wreszinski, J. Stat. Phys. **58**, 45 (1990).
- [33] C. Hamer, G. Quispel, and M. Batchelor, J. Phys. A: Math. Gen. **20**, 5677 (1987).
- [34] J. Sirker and M. Bortz, J. Stat. Mech. **2006**, P01007 (2006).
- [35] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (New York, McGraw-Hill, 1953).
- [36] For the connection between the $U(1)$ flux and the DM interaction, see Supplemental Material.
- [37] C.-N. Yang and C.-P. Yang, Phys. Rev. **150**, 321 (1966).
- [38] I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
- [39] We have checked numerically for small system sizes that this relation holds for any $\Phi \in (-\pi, \pi)$.
- [40] This can be seen by noting that
- $$[\prod_{l=1}^N 2\hat{S}_l^x]^{-1} \hat{\mathcal{H}}(\Phi) [\prod_{l=1}^N 2\hat{S}_l^x] = \hat{\mathcal{H}}(-\Phi).$$
- [41] N. Aiba and K. Nomura, Phys. Rev. B **102**, 134435 (2020).
- [42] For the data of the other order weights under the magnetic field, see Supplemental Material.
- [43] H. de Vega and F. Woynarovich, Nucl. Phys. B **251**, 439 (1985).
- [44] C. J. Hamer, J. Phys. A: Math. Gen. **19**, 3335 (1986).
- [45] F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, Phys. Rev. Lett. **58**, 771 (1987).
- [46] F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, Annals Phys. **182**, 280 (1988).
- [47] F. Woynarovich and H.-P. Eckle, J. Phys. A: Math. Gen. **20**, L97 (1987).
- [48] S. Lukyanov, Nucl. Phys. B **522**, 533 (1998).
- [49] T. Giamarchi, *Quantum Physics in One Dimension*, International Series of Monographs on Physics (Clarendon Press, 2003).
- [50] J. Sirker, Int. J. Mod. Phys. B **26**, 1244009 (2012).
- [51] Although we have excluded non-generic values of γ , the leading behavior of the finite size correction is the same as Eqs. (9) and (10) even for these γ except for $\gamma = \pi l/(l+2)$ ($l \in \mathbb{N}$). The analysis of the exceptional cases requires some additional care and will be discussed elsewhere.
- [52] J. Sirker, R. G. Pereira, and I. Affleck, Phys. Rev. B **83**, 035115 (2011).
- [53] A. Klümper, M. T. Batchelor, and P. A. Pearce, J. Phys. A: Math. Gen. **24**, 3111 (1991).