

# Spin-Current Autocorrelations from Single Pure-State Propagation

Robin Steinigeweg,<sup>1,\*</sup> Jochen Gemmer,<sup>2,†</sup> and Wolfram Brenig<sup>1,‡</sup>

<sup>1</sup>*Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany*

<sup>2</sup>*Department of Physics, University of Osnabrück, D-49069 Osnabrück, Germany*

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We demonstrate that the concept of quantum typicality allows for significant progress in the study of real-time spin dynamics and transport in quantum magnets. To this end, we present a numerical analysis of the spin-current autocorrelation function of the antiferromagnetic and anisotropic spin-1/2 Heisenberg chain as inferred from propagating only a *single* pure state, randomly chosen as a “typical” representative of the statistical ensemble. Comparing with existing time-dependent density-matrix renormalization group (tDMRG) data, we show that typicality is fulfilled extremely well, consistent with an error of our approach, which is perfectly under control and vanishes in the thermodynamic limit. In the long-time limit, our results provide for a new benchmark for the enigmatic spin Drude weight, which we obtain from chains as long as  $L = 33$  sites, i.e., from Hilbert spaces of dimensions almost  $\mathcal{O}(10^4)$  larger than in existing exact-diagonalization studies.

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*Introduction.* Understanding relaxation and transport dynamics in quantum many-body systems is one of the most ambitious aims of condensed-matter physics and is experiencing an upsurge of interest in recent years, both experimentally and theoretically. On the one hand, the advent of ultracold atomic gases raises challenging questions about the thermalization of isolated many-body systems [1]. On the other hand, future information technologies such as spintronics call for a deeper insight into transport processes of quantum degrees of freedom such as spin excitations. While spin transport in conventional nano-systems [2–5] is inevitably linked to itinerant charge-carrier dynamics, Mott-insulating quantum magnets allow for pure spin currents, opening new perspectives in quantum transport. Magnetic transport in one-dimensional (1D) quantum magnets has attracted considerable attention in the past decade due to the discovery of very large magnetic heat-conduction [6–8] and long nuclear magnetic relaxation times [9, 10]; so far, however, pure spin transport remains to be observed experimentally.

Within the large body of theoretical work accumulated [11–33], the dissipation of magnetization currents is a key issue. This issue has been studied extensively at zero momentum and frequency in connection with the well-known spin Drude weight: It is the non-decaying contribution of the spin current and signals dissipationless transport. A paradigmatic model in these studies is the Heisenberg chain with periodic boundary conditions ( $\hbar = 1$ ),

$$H = J \sum_{r=1}^L (S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z), \quad (1)$$

where  $S_r^{x,y,z}$  are the components of spin-1/2 operators at site  $r$ .  $L$  is the total number of sites,  $J > 0$  the antiferromagnetic exchange coupling constant, and  $\Delta$  the anisotropy.

At zero temperature,  $T = 0$ , early work [11] showed that the Drude weight is finite in the gapless regime  $\Delta \leq 1$  (metal) but vanishes in the gapped case  $\Delta > 1$  (insulator). At finite temperature,  $T > 0$ , Bethe-Ansatz results [12, 13] support a qualitatively similar picture, but with a disagreement at the isotropic point  $\Delta = 1$ . Recent progress in combining quasi-local conservation laws and the Mazur’s inequality has led to a rigorous lower bound to the Drude weight at high temperatures  $T \gg J$  [14, 15], which is very close to the Bethe-Ansatz solution but still allows for a vanishing Drude weight at  $\Delta = 1$ .

Numerically, a large variety of sophisticated methods has been applied to spin transport in Heisenberg chains, including full exact diagonalization (ED) [16–20],  $T > 0$  Lanczos [21], quantum Monte-Carlo [24, 25], wave-packet propagation by tDMRG [26], real-time correlator calculations [27–29], and Lindblad quantum master equations [30]. The Drude weight, however, is only available from ED and tDMRG. Since, as of today, ED is restricted to chains of length  $L \sim 20$ , the long-time (low-frequency) regime is still governed by finite-size effects and intricate extrapolation schemes to the thermodynamic limit have been invoked, with different results depending on details – including remarkable differences between even and odd  $L$  [18], or grand-canonical and canonical ensembles [28]. Alternatively, tDMRG is exceedingly more powerful w.r.t. system size and chains with  $L \sim 200$  are accessible; however, the method is still confined to a maximum time scale depending on  $\Delta$  [27–29], with an ongoing progress to increase this scale [34]. As of today, the latter scale is too short for a reliable extraction of the Drude weight at the isotropic point  $\Delta = 1$  [28].

Therefore, no consistent picture on the Drude weight for  $T \neq 0$  is available at  $\Delta \sim 1$ . It is worth mentioning that, apart from Drude weights indicating ballistic dynamics, steady-state bath scenarios [30] and classical simulations [31] suggest super-diffusive dynamics at  $T \gg J$ ,

while bosonization predicts diffusion at sufficiently low temperatures  $J \gg T > 0$  [32].

In this situation, our Letter takes a fresh perspective, rooted in quantum statistical physics and leading to a surprisingly simple, yet very powerful numerical approach to evaluate finite-temperature time-dependent correlation functions in general and the dynamics of spin currents in the Heisenberg chain in particular. This approach is intimately related to the emergent concept of quantum typicality [35–42] and overcomes the restriction of ED to small system sizes without a restriction to short times. Specifically, in this Letter, we will unveil that (i) quantum typicality is fulfilled extremely well for system sizes  $L \sim 30$  down to temperatures  $T/J = 0.5$  and that (ii) our approach yields exact information on an extended time window in the thermodynamic limit. Furthermore, because our approach is not restricted to short times, we are able to (iii) calculate the Drude weight for chains as long as  $L = 33$  sites, i.e., for Hilbert spaces almost  $\mathcal{O}(10^4)$  times larger than in present ED at  $L \leq 20$ . Thus, our results (iv) severely constrain any remaining speculations on the long-standing issue of the finite-temperature spin Drude weight of the isotropic Heisenberg chain.

*Numerical approach.* The well-known spin-current operator  $j = J \sum_r (S_r^x S_{r+1}^y - S_r^y S_{r+1}^x)$  follows from the continuity equation [17]. Within the framework of linear response theory, we are interested in the autocorrelation function at inverse temperatures  $\beta = 1/T$  ( $k_B = 1$ ),

$$C(t) = \frac{\langle j(t)j \rangle}{L} = \frac{\text{Tr}\{e^{-\beta H} j(t)j\}}{L \text{Tr}\{e^{-\beta H}\}}, \quad (2)$$

where the time argument of  $j$  has to be understood w.r.t. the Heisenberg picture,  $j = j(0)$ , and  $C(0) = J^2/8$  at high temperatures  $\beta \rightarrow 0$ . For the validity of linear response theory, see Refs. 22 and 23.

The basic idea underlying our numerical approach is to replace the trace  $\text{Tr}\{\bullet\} = \sum_n \langle n | \bullet | n \rangle$  by a scalar product involving a single pure state  $|\psi\rangle$  drawn at random. More precisely, following the concept of quantum typicality [35–38],  $|\psi\rangle$  is drawn at random from a probability distribution which is invariant under all possible unitary transformations in Hilbert space (Haar measure [40]). Drawing such a random pure state  $|\psi\rangle$  and abbreviating  $|\psi_\beta\rangle = e^{-\beta H/2} |\psi\rangle$ , we can approximate the autocorrelation function by [40–42]

$$C(t) = \frac{\langle \psi_\beta | j(t)j | \psi_\beta \rangle}{L \langle \psi_\beta | \psi_\beta \rangle} + \mathcal{O}\left(\frac{\sqrt{\langle j(t)j j(t)j \rangle}}{L \sqrt{d_{\text{eff}}}}\right), \quad (3)$$

where the second term is a random variable with zero mean and standard deviation  $\propto 1/\sqrt{d_{\text{eff}}}$ , with  $d_{\text{eff}}$  as the effective dimension of the Hilbert space. In the limit of high temperatures  $\beta \rightarrow 0$ ,  $d_{\text{eff}} = 2^L$ . Hence, if the chain length  $L$  is increased, the error decreases exponentially with  $L$  and the approximation becomes accurate rather quickly. At arbitrary temperatures,

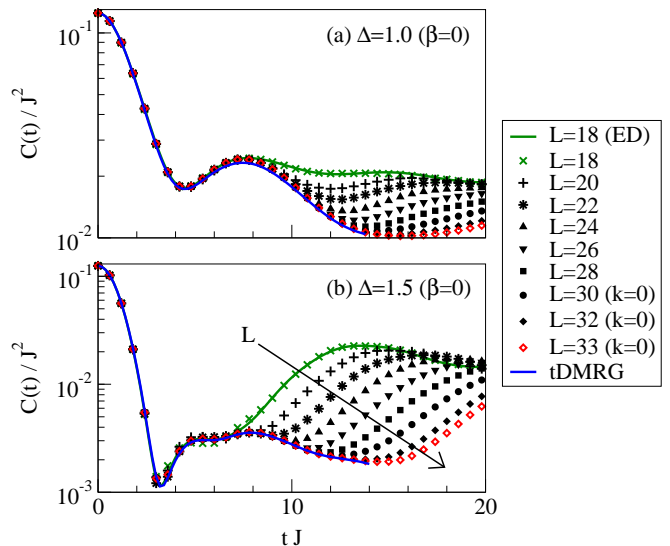


FIG. 1. (color online) Spin-current autocorrelation function  $C(t)$  at  $\beta \rightarrow 0$  for (a)  $\Delta = 1.0$  and (b)  $\Delta = 1.5$ , numerically obtained for  $L = 18$  using the full statistical ensemble (green curve) and larger  $L \geq 18$  using a single pure state (symbols), shown in a semi-log plot. The very high accuracy is illustrated by comparing to available tDMRG data for  $L = 200$  [27, 29] (blue curve).

$d_{\text{eff}} = \text{Tr}\{e^{-\beta(H-E_0)}\}$  is the partition function and  $E_0$  the ground-state energy. This expression also scales exponentially with  $L$  [43], rendering the approximation exact once again for  $L \rightarrow \infty$ , however less quickly. In any case, the error in Eq. (3) can be reduced additionally by averaging over several random pure states  $|\psi\rangle$ .

The central advantage of Eq. (3) is that the first term on the r.h.s. can be evaluated without diagonalization of the Hamiltonian. This can be seen by introducing two pure states: The first is  $|\Phi_\beta(t)\rangle = e^{-iHt - \beta H/2} |\psi\rangle$  and the second is  $|\varphi_\beta(t)\rangle = e^{-iHt} j e^{-\beta H/2} |\psi\rangle$ . Then,

$$\langle \psi_\beta | j(t)j | \psi_\beta \rangle = \langle \Phi_\beta(t) | j | \varphi_\beta(t) \rangle. \quad (4)$$

The  $t(\beta)$  dependence of the two states can be calculated by iterating in real (imaginary) time using, e.g., Runge-Kutta [42, 43] or Chebyshev [44, 45] schemes. We find that a fourth order Runge-Kutta (RK4) scheme with a small discrete time step  $\delta t J = 0.01 \ll 1$  is sufficient. Although the algorithm does not require to save Hamiltonians and observables in memory, it is convenient w.r.t. run time to do so, requiring only sparse matrices with  $L 2^L \ll 2^{2L}$  elements. It is further convenient to choose the random pure state  $|\psi\rangle$  from the common eigenbasis of symmetries, e.g., translation invariance and rotations about the  $z$  axis, taking full advantage of the block structure of the Hamiltonian in that basis. In this way, we are able to treat chains as long as  $L = 33$ , where the full Hilbert-space dimension is huge:  $2^{33} \approx 10^{10}$ . (In that case the dimension of the largest symmetry subspace is  $3.5 \cdot 10^7$ .) It is worth mentioning that symmetries, in

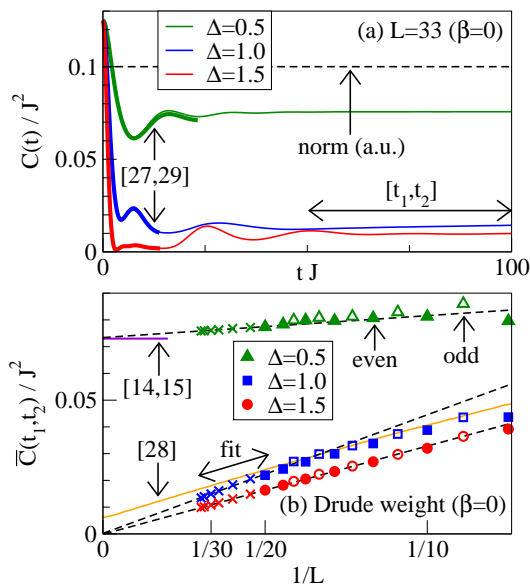


FIG. 2. (color online) (a) Long-time limit of the spin-current autocorrelation function  $C(t)$  at  $\beta \rightarrow 0$  for  $\Delta = 0.5, 1.0,$  and  $1.5$ , numerically obtained using a single pure state (thin solid curves). The well-conserved norm is indicated (thin dashed curve). Available tDMRG data for  $L = 200$  [27, 29] are shown (thick solid curves). (b) Finite-size scaling of the spin Drude weight, extracted in the time interval  $[t_1 J, t_2 J] = [50, 100]$  (closed [open] symbols for even [odd]  $L$ ;  $L \leq 20$ : full statistical ensemble; and  $L \gg 20$ : single pure state). Simple  $1/L$  fits to large  $20 \leq L \leq 33$  are depicted (dashed lines), and at  $\Delta = 1.0$  the odd-site fit to  $L \leq 19$  performed in Ref. 28 (solid curve). At small  $\Delta = 0.5$ , T. Prosen’s strict analytic lower bound [14, 15] is indicated (horizontal line).

combination with massive parallelization on super computers [45], have the potential to reach  $L \sim 40$  in the future.

*Results.* Let us begin with the high-temperature limit  $\beta \rightarrow 0$  and systems of intermediate size  $L = 18$ . In Fig. 1 (a) we first compare the exact autocorrelation function in Eq. (2), obtained from ED, at the isotropic point  $\Delta = 1$  with the approximation in Eq. (3), obtained from RK4, using a single pure random state  $|\psi\rangle$ . At all times, the agreement between Eq. (2) and Eq. (3) is remarkably good. This agreement is underlined even more through our usage of a log  $y$  axis, emphasizing relative rather than only absolute accuracy. In view of this agreement, and with any remaining error decreasing exponentially with  $L$ , we can safely consider the Eq. (3) as almost exact for  $L > 18$  and we will neglect any averaging over random pure states  $|\psi\rangle$ . By increasing  $L$  in Fig. 1 (a), we show that the curve of the autocorrelation function gradually converges in time towards the thermodynamic limit. For the maximum  $L = 33$  the curve is converged up to times  $tJ \sim 15$  with no visible finite-size effects in the semi-log plot. Note that for the three largest  $L \geq 30$  we restrict ourselves to a single translation subspace to reduce com-

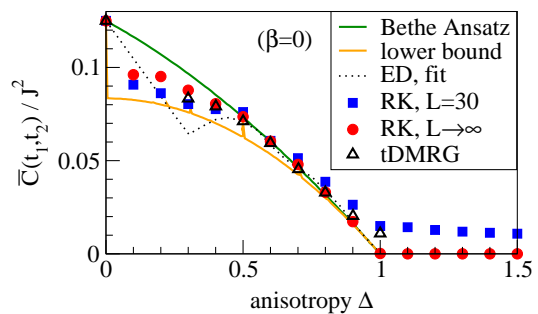


FIG. 3. (color online) High-temperature Drude weight  $\bar{C}$  from single pure-state propagation w.r.t. the anisotropy  $\Delta$  (closed symbols), compared to the thermodynamic Bethe-Ansatz [12], T. Prosen’s strict analytic lower bound [14, 15], the fit to ED at zero magnetization and odd sites performed in Ref. 18, and tDMRG [27] (see also Ref. 28 for a different point of view on the tDMRG data point at  $\Delta = 1$ ).

putational effort at high temperatures  $\beta \rightarrow 0$ , see also Ref. [18]. Next, we compare to existing tDMRG data for  $L = 200$  [27]. It is intriguing to see that our results agree up to very high precision. On the one hand, this observation is the most convincing demonstration of quantum typicality so far. On the other hand, it indicates that our approach yields exact information on an extended time window in the thermodynamic limit. These latter points are two main results of this Letter.

In Fig. 1 (b) we show a second calculation for a larger anisotropy  $\Delta = 1.5$ . Clearly,  $C(t)$  decays to almost zero rapidly. However, a small long-time tail remains. This tail has been anticipated already on the basis of ED at  $L = 20$  [19], leading to a positive correction to the diffusion constant from perturbation theory [20]. Note that the tail is not connected to the Drude weight [29], as discussed in more detail later.

Next we study the long-time limit. In Fig. 2 (a) we show  $C(t)$  for  $\beta \rightarrow 0$  and  $\Delta = 0.5, 1.0,$  and  $1.5$ . We also depict the norm of  $|\Phi_\beta(t)\rangle$ , which is practically constant, as  $|\varphi_\beta(t)\rangle$  is also. This clearly demonstrates that the RK4 scheme works properly at such long times. This figure also proves (i) the saturation of  $C(t)$  at rather long times  $tJ \sim 50$  and that (ii) we can hardly infer the saturation value from our short-time data in Fig. 1.

Because the long-time limit is governed by finite-size effects, we are now going to perform a proper finite-size scaling in terms of the Drude weight. To this end, let us define the Drude weight  $\bar{C} = 1/(t_2 - t_1) \int_{t_1}^{t_2} C(t) dt$  as the average over the time interval  $[t_1 J, t_2 J] = [50, 100]$ . The Drude weight has been extracted similarly in Ref. 19, yielding the correct zero-frequency value [17].

In Fig. 2 (b) we depict the resulting Drude weight vs. the inverse length  $1/L$  for anisotropies  $\Delta = 0.5, 1.0,$  and  $1.5$ . While for  $L > 20$  we extract the Drude weight from the approximation in Eq. (3) (denoted by crosses), we use the exact expression in Eq. (2) for  $L \leq 20$  (denoted

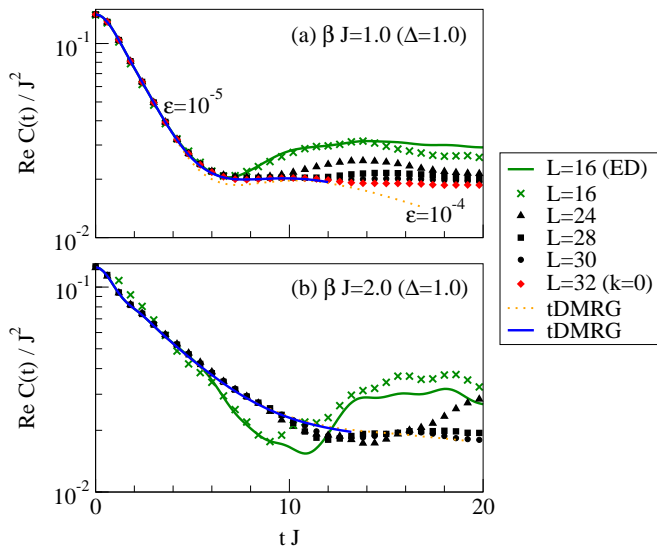


FIG. 4. (color online) Spin-current autocorrelation function  $C(t)$  for  $\Delta = 1.0$  at (a)  $\beta J = 1.0$  and (b)  $\beta J = 2.0$ , numerically obtained for  $L = 16$  using the full statistical ensemble (green curve) and larger  $L \geq 16$  using a single pure state (symbols), shown in a semi-log plot. Available tDMRG data for  $L = 200$  [27, 28] are depicted for two values of the discarded weight  $\epsilon$  (blue and orange curve).

by other symbols), to avoid typicality errors at small  $L$ . We also indicate the results of  $1/L$  fits, solely based on data points for  $L \geq 20$ , to avoid the influence of even-odd effects and the need of  $(1/L)^{i>1}$  corrections at small  $L$ . Remarkably, for  $\Delta = 0.5$ , the resulting fit is close to *all* data points. Extracting the thermodynamic limit  $L \rightarrow \infty$  from the fits, we find a non-zero Drude weight in convincing agreement with the rigorous lower bound of Refs. 14 and 15. The situation is rather similar for  $\Delta = 1.5$  but with a vanishing Drude weight for  $L \rightarrow \infty$ , consistent with previous work [17]. Certainly, the isotropic point  $\Delta = 1.0$  is most interesting. Here, the  $L \geq 20$  fit is not close to that obtained from only small  $L < 20$ . In fact, the extrapolation yields much smaller values for the Drude weight than the finite values suggested in previous works, based on either smaller  $L$  [17, 28] or shorter  $t$  [27] (see also Ref. 28 for a detailed discussion). In fact, our approach is consistent with a vanishing Drude weight for  $L \rightarrow \infty$ . This is another main result of this Letter.

In Fig. 3 we summarize the finite-size values for the Drude weight for fixed  $L = 30$  and various anisotropies  $0 \leq \Delta \leq 1.5$ . Additionally, we indicate the extrapolated values for  $L \rightarrow \infty$  using fits to, e.g., only even sites, which is important closer to  $\Delta = 0$ . Remarkably, all extrapolated values lie above the rigorous lower bound of Refs. 14 and 15 and, in the anisotropy range  $0.4 \lesssim \Delta \leq 1.5$ , also agree with the Bethe-Ansatz solution of Ref. [12]. They further agree with an alternative extrapolation on the basis of small  $L$  [18], using a different statistical ensemble and only odd sites. In the *vicinity* of  $\Delta = 0$ , where relax-

ation is slow, our definition of the Drude weight in terms of  $\bar{C}$  may include low-frequency contributions. Still we lie above the lower bound but observe deviations from the Bethe-Ansatz solution. These deviations are well-known to occur in numerical studies using finite systems [18], due to the very high degeneracy at  $\Delta = 0$ .

Finally, we turn to finite temperatures  $\beta \neq 0$ . Clearly, our numerical approach has to break down for  $\beta \rightarrow \infty$ , i.e.,  $T \rightarrow 0$ , due to the reduction of the effective Hilbert space dimension in Eq. (3). Moreover, also the exact expression in Eq. (2) is governed by large finite-size effects for  $\beta J \gg 2$ , at least at  $L \sim 30$  [21]. Thus, for a numerical approach to  $L \sim 30$ , reasonable temperatures are  $\beta J \sim 2$ . For this range of  $\beta$  the approximation is still justified and averaging is crucial for  $\beta \gg 2$  only.

In Fig. 4 (a) and (b) we compare the approximation in Eq. (3), calculated by RK4, and the exact expression in Eq. (2), calculated by ED, for a system of intermediate size  $L = 16$  and the two lower temperatures  $\beta J = 1$  and 2, with the focus on  $\Delta = 1$ . While deviations appear at  $\beta J = 2$ , these deviations manifest as random fluctuations rather than systematic drifts and may be compensated by additional averaging over several pure states. However, one can expect that these deviations disappear for significantly larger  $L$ . Again, we prove this by comparing with existing tDMRG data for  $L = 200$  [27, 28]. This result illustrates the power of our numerical approach at finite temperatures. Moreover, taking into account (i) the simple structure of the curve, (ii) the semi-log plot, and (iii) the combination of tDMRG with our numerical approach, Fig. 4 (a) is very indicative to non-zero Drude weights at  $\beta \neq 0$ , in contrast to  $\beta \rightarrow 0$ , which is another main result of this Letter.

*Conclusion.* We used the emergent concept of quantum typicality to obtain an alternative and innovative numerical approach to several timely issues regarding spin transport in anisotropic and antiferromagnetic spin-1/2 Heisenberg chains. We showed that quantum typicality is fulfilled extremely well for system sizes  $L \sim 30$  down to temperatures  $T/J = 0.5$ . Because our approach is not restricted to short times, we were able to calculate the Drude weight for chains as long as  $L = 33$  sites. This enabled us to drastically narrow down any options for the long-standing question of Drude weights in the isotropic Heisenberg chain, which we find to be very small or vanishing at high temperatures. We hope that in the future our approach complements other numerical techniques in a much broader context, including problems with few symmetries [46] and/or in two dimensions [47]. In non-integrable systems we expect very small finite-size effects for the huge Hilbert spaces reachable by our approach.

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\* r.steinigeweg@tu-bs.de

† jgemmer@uos.de

‡ w.brenig@tu-bs.de

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