Finite-temperature Drude weight within the anisotropic Heisenberg chain

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Finite-temperature Drude weight (spin stiffness) $D(T)$ is evaluated within the anisotropic spin-$1/2$ Heisenberg model on a chain using the exact diagonalization for small systems. It is shown that odd-side chains allow for more reliable scaling and results, in particular if one takes into account corrections due to low-frequency finite-size anomalies. At high $T$ and zero magnetization $D$ is shown to scale to zero approaching the isotropic point $\Delta = 1$. On the other hand, for $\Delta > 2$ at all magnetizations $D$ is nearly exhausted with the overlap with the conserved energy current. Results for the $T$-variation $D(T)$ are also presented.

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I. INTRODUCTION

It has by now become evident that many-body (MB) quantum systems of interacting particles behave with respect to transport quite differently if they are either integrable or non-integrable\textsuperscript{[1, 2]}. In integrable systems the anomalous response shows up in a possibility of finite-temperature stiffness (Drude weight) $D(T) > 0$\textsuperscript{[3]}, both the charge (or spin) and the thermal one\textsuperscript{[5]}, indicating the dissipationless d.c. transport at $T > 0$. The prototype model for this phenomenon is the anisotropic spin-$1/2$ Heisenberg model on a chain, equivalent to the one-dimensional (1D) $t$-$V$ model of spinless fermions with nearest neighbor repulsion. Within this model one of the conserved quantities is the energy current $j_E$ leading to the singular but trivial thermal dynamical conductivity linear response \[\kappa(\omega) = D_T\delta(\omega).\] On the other hand, the spin current $j$ and the corresponding dynamical spin conductivity (diffusivity) $\sigma(\omega)$ at $T > 0$ is still the subject of very active theoretical investigations and debate.

In the case of a nonvanishing projection of the spin current $j$ on local conserved quantities $Q_n$, the Mazur inequality offers a firm proof of finite $D(T \neq 0) > 0$\textsuperscript{[5]} in the thermodynamic limit. Still, at zero magnetization, i.e., at the total spin $S^z = 0$ the overlap with all $Q_n$ vanishes independent of the anisotropy $\Delta$\textsuperscript{[5]}. To employ the same argument one possible path is to construct more general nonlocal conserved quantities\textsuperscript{[6, 7]} which should be further explored.

The (original) alternative formulation via the MB level dynamics induced in a 1D ring via an external flux\textsuperscript{[3, 4]} offers a qualitative understanding and is the starting point for numerical calculations using the full exact diagonalization (ED) method\textsuperscript{[8–11]}. The latter so far did not eliminate disagreement on several questions: a) is $D$ a monotonous function of $\Delta$ at fixed $S^z$\textsuperscript{[10]}, b) does $D(T > 0)$ vanish on approaching the isotropic point $\Delta = 1, S^z = 0$\textsuperscript{[8, 12]}, c) which if any analytical result, obtained via the Thermodynamic Bethe Ansatz\textsuperscript{[13, 15]}, is correct and compatible with numerical investigations.

In the following we present results of the numerical study for $D(T)$ as obtained using the ED and the scaling for small systems. In contrast to previous works\textsuperscript{[9, 10]} we perform the study within the canonical ensemble which offers much faster convergence with the chain size $L$, at least approaching the isotropic point $\Delta \sim 1, S^z \sim 0$. To avoid quite singular behavior of even-lengths chains, we study spin systems with odd $L$. In particular, we pay the attention to possible low-frequency contributions in the dynamical conductivity $\sigma(\omega)$ which can give an insight into anomalies around commensurate $\Delta = \cos(\pi/\nu)$ with integer $\nu$, e.g., at $\Delta < 0.5$.

The paper is organized as follows: In Sec. II we present the model and Drude weight $D$ as zero frequency contribution to dynamical conductivity. We shortly also describe numerical method used to analyse it. Our results are presented in Sec. III. First we investigate the high-temperature limit $C = TD$, where we emphasize the low-frequency contributions which can mask the correct result. We show also that within Ising-type regime $\Delta > 1$ the Drude weight calculated via the overlap with the conserved energy current gives nearly perfect results. Finally we focus on the temperature variation of $D(T)$.

II. DRUDE WEIGHT

We study the anisotropic $S = 1/2$ Heisenberg model on a chain with $L$ sites and periodic boundary conditions

$$H = J \sum_{i=1}^{L} (S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + \Delta S_z^i S_z^{i+1}),$$

where $S_i^\alpha$ are component of the $S = 1/2$ spin operators. In order to define the Drude weight (spin stiffness) $D$ it is convenient to map the model\textsuperscript{[11]} via the Jordan-Wigner transformation onto the $t$-$V$ model of interacting spinless fermions adding a fictitious magnetic flux $\Phi = L\phi$ through the ring\textsuperscript{[4, 14]}, entering the hopping matrix elements,

$$H = t \sum_i (e^{i\phi} c_i^\dagger c_{i+1} + \text{h.c.}) + V \sum_i \left( n_i - \frac{1}{2} \right) \left( n_{i+1} - \frac{1}{2} \right),$$

\begin{equation}
\begin{array}{l}
n_i = c_i^\dagger c_i, \quad t = J/2 \quad \text{and} \quad V = 2t \Delta. \quad \text{Here we consider only chains with odd number of fermions $N$ to avoid additional}
\end{array}
\end{equation}
boundary fermionic sign and other finite-size effects discussed in more detail below. In the following we use everywhere \( J = 1 \) in order to facilitate the comparison with the majority of previous works and references \([9, 10, 13]\). Note that relevant parameters are now the total spin \( S_z \) and magnetization \( s = S_z/L \) or the fermion density or band filling \( n = N/L = s + 1/2 \).

Via the corresponding spin (particle or charge within the fermionic model) current

\[
j = t \sum_i (i e^{ij} \hat{c}_i \hat{c}_{i+1} + \text{h.c.}),
\]

one can express the dynamical (spin) conductivity at general temperature \( T > 0 \) as

\[
\sigma(\omega) = 2\pi D \delta(\omega) + \sigma_{\text{reg}}(\omega),
\]

where the regular part \( \sigma_{\text{reg}}(\omega) \) expressed in terms of eigenstates \( |n\rangle \) and eigenenergies \( \epsilon_n \),

\[
\sigma_{\text{reg}}(\omega) = \frac{\pi}{L} \sum_{\epsilon_n \neq \epsilon_m} \sum_{p_n} |\langle n| jm\rangle|^2 \delta(\epsilon_n - \epsilon_m - \omega),
\]

while the dissipationless component with the Drude weight (spin stiffness) \( D \) can be related to the flux dependence of MB states \([3]\), in analogy with the original formulation by Kohn \([14]\)

\[
D = \frac{1}{2L} \sum_n p_n \frac{\partial^2 \epsilon_n(\phi)}{\partial \phi^2},
\]

where \( p_n = \exp(-\beta \epsilon_n)/Z \) are corresponding Boltzmann factors.

The relation (6) is convenient for the ED numerical evaluation of \( D(T) \) in small systems, since it only requires the calculation of eigenvalues \( \epsilon_n(\phi) \). Finally we are interested in the result within the thermodynamic limit \( T \to \infty \) at fixed \( T \) and magnetization \( s \) (filling \( n \) ), hence several strategies to obtain the thermodynamic value are possible. Since we mostly consider the high-\( T \) limit (allowing for most accurate ED results in small systems) and ED sizes are quite limited \( L \leq 21 \), we perform the canonical calculation at total spin \( S_z^c \) (fermion number \( N \)). The grand canonical evaluation at available \( L \) and high \( T \) has a very broad distribution of \( N \), leading to overestimates of \( D \) (or at least its slow convergence with \( L \)) in the vicinity of the isotropic phase, i.e., at \( s \sim 0, \Delta \sim 1 \).

On the other hand, also results with even \( L \) show deficiencies \([10]\). Treating in Eq. (5) the flux \( \phi \) as parameter, corresponding \( D(\phi, T \gg 0) \) show strong anomaly at \( \phi \to 0 \) for even \( L \) and even \( N \) due to the particle-hole symmetry and degeneracy of MB levels. In addition, even-\( L \) systems give at odd \( N \) considerably lower values for \( D \) at \( \Delta < 1 \) and small \( L \) \([10]\) (an origin could be also particle-hole symmetry absent at odd \( L \)) remedied presumably only at much larger \( L \). To avoid these complications, we in the following consider only systems with odd \( L = 5 - 21 \) (for \( L = 21 \) only one \( k \)-vector due to very high CPU requirements) which reveal much weaker and more regular \( D(\phi) \) dependence.

III. RESULTS

A. High-Temperature Limit.

In the following we mostly concentrate on the limit \( T \to \infty \), expecting that obtained results are quite generic and qualitatively similar at any \( T > 0 \). Since for \( T \to \infty \), \( D(T) \) scales as \( 1/T \) the relevant and nontrivial quantity is \( C = TD(T) \), representing also the limiting value of the current-current correlation function \( C = C_{jj}(t \to \infty) \) \([5]\). Let us first consider the most delicate zero-magnetization \( s = 0 \) (half-filling \( n = 1/2 \) case). Since we choose odd \( L \), the actual calculations are performed for closest odd \( N = (L \pm 1)/2 \). Results for \( C \) vs. \( 1/L \) for all odd \( L = 5 - 19 \) are presented for different \( \Delta \) in Fig. 1. Several conclusions can be drawn directly from obtained results: a) Both values as well as the scaling with \( L \) are qualitatively different between \( \Delta \geq 1 \) and \( \Delta < 1 \). It is evident that for \( \Delta \geq 1 \) the only consistent limit appears to be \( C = 0 \). b) There are some visible anomalies near \( \Delta < 0.5 \) which indicate on a nonuniform dependence of \( C(\Delta) \) \([10]\) and in particular different scaling \( L \to \infty \) which we discuss in more detail below.

In order to resolve the origin of the deviations of \( C \) at \( \Delta < 0.5 \) as well as of quite regular convergence of results for other values of \( \Delta \) we investigate the dynamical \( \sigma(\omega) \), shown conveniently also in the integrated form for \( T \to \infty \),

\[
I(\omega) = C + \frac{T}{\pi} \int_0^\omega \sigma_{\text{reg}}(\omega')d\omega',
\]

consistent with the sum rule

\[
I(\omega \to \infty) = T c_{\text{kin}} = -T(H_{\text{kin}})/L,
\]

where \( H_{\text{kin}} \) is the kinetic-energy part in the model \([2]\). \( c_{\text{kin}} \) can be evaluated exactly in the \( \beta \to 0 \) limit, even for finite \( L \).
and fixed $N$,

$$
e_{\text{kin}} = \frac{\beta J^2}{4} \frac{N}{L} \left(1 - \frac{N - 1}{L - 1}\right)
$$

(9)

In Fig. 2 we present characteristic results for $\sigma_{\text{reg}}(\omega)$ as well as $I(\omega)$ (inset) for two commensurate values $\nu = 3, 6$, i.e., $\Delta = 0.5, \sqrt{3}/2 = 0.866$, respectively. We note that for $\Delta = 0.5$ the incoherent part in $\sigma_{\text{reg}}(\omega)$ is quite $L$-independent in a broad range $L = 13 - 21$ and consequently the convergence of obtained Drude weight $C$ vs. $1/L$ is very stable. Less obvious case is $\Delta = 0.866 (\nu = 6)$ being already closer to the critical value $\Delta = 1$. The incoherent $\sigma_{\text{reg}}(\omega)$ reveals here a low-$\omega$ contribution whereby the peak is shifting as with $1/L$ as observed even more pronounced for $\Delta > 1$ [16]. However, in the present case the peak intensity as well diminishes with $L$ (a closer inspection reveals that the peak $\omega_p$ also vanishes here faster than $1/L$) so that the integrated $I(\omega)$ in Fig. 2b appears to have well defined limit $C = I(\omega \to 0)$.

In Fig. 3 we present $I(\omega)$ for $\Delta = 0.25$ characteristic for the regime $\Delta < 0.5$. We note that the high-$\omega$ part is quite $L$-independent (note that for $L=21$ we calculate only one $k$-vector, which influences slightly the sum rule $I(\omega \to \infty)$) similar to results for $\Delta = 0.5$ in Fig. 2a. However, there is also a well visible anomalous low-$\omega$ contribution at $0.02 < \omega < 0.08$ (see the inset). The peak in $\sigma(\omega)$ (as obtained from $I(\omega)$ in the inset of Fig. 3) appears to shift towards $\omega_p = 0$ somewhat faster than $1/L$ (approximate fit $\omega_p \sim 1.342/L - 0.017$) whereas its weight in $I(\omega)$ increases with the system size. This deviation can be counted as an additional contribution to effective $\delta C$. This is, e.g., in contrast to case $\Delta = 0.866$, where the intensity decreases with $L$ (Fig. 2). Although the origin of the low-$\omega$ anomaly is not well understood it seems that it is absent for commensurate values of $\Delta = \cos(\pi/\nu)$ which possess additional degeneracies [13].

Results for $C$ vs. $1/L$ as in Fig. 1 can be used to extrapolate to the thermodynamic value $C$ where we use the extrapolation $C(L) = C + \alpha/L + \zeta/L^2$. Obtained results for $C(\Delta)$ are presented in Fig. 4. On the other hand, one can correct $C(L)$ with the low-$\omega$ contribution $\tilde{C}(L) = C(L) + \delta C(L)$ and get modified extrapolation $\tilde{C}$, also presented in Fig. 4. We can now compare the results with the analytical result obtained via Thermodynamic Bethe Ansatz (TBA) [13, 15].

$$
C = \frac{\gamma - \frac{1}{2} \sin(2\gamma)}{16\gamma}, \quad \Delta = \cos(\gamma),
$$

(10)

the validity of which has been still questioned [12, 15]. We note that the agreement of the analytical form (10) with the corrected numerical $\tilde{C}$ is very satisfactory for $s = 0$ within the whole regime of $\Delta$.

Let us now turn to the dependence of $C$ on magnetization $s$ (filling $n$). It is evident that one gets $C = 0$ within the Ising-type regime $\Delta > 1$ only for $s = 0$. Results for $C$ at $\Delta = 1.7$ and $\Delta = 3$ are shown in Fig. 5 for fixed $L = 19$ and all available $S_z$. It is indicative that $C(s)$ are nearly equal for both $\Delta > 1$. To go beyond the finite-size results one can also perform the scaling to $L \to \infty$ analogous to $n = 1/2$ case which is possible, e.g., for $s = 1/4$ (taking into account results for $L = 5 - 25$) and $s = 1/3$ (with results for $L = 9 - 21$). Corresponding results for the extrapolated $C$ are also plotted in Fig. 5, confirming that $C(s)$ become essentially universal.
for $\Delta > 1$.

It has been already observed in Ref.[5] that within the Ising regime $\Delta > 1$ the Drude weight can be via the Mazur inequality well exhausted with the overlap onto the simplest nontrivial local conserved quantity $Q_3 = j_E$ representing the energy current. At $T \rightarrow \infty$ this overlap can be evaluated exactly leading to

$$C_3 = \frac{1}{2L} \left( \frac{JQ_3}{Q_3^2} \right)^2 = \frac{\Delta^2 s^2(1 - 4s^2)}{1 + 2\Delta^2(1 + 4s^2)}.$$  \hspace{1cm} (11)

From Fig. 5 we see that the agreement between the approximate $C_3$, Eq.(11), and the extrapolated $C$ is nearly perfect for large $\Delta \gg 1$, e.g., $\Delta = 3$, while for $\Delta = 1.7$ the value $C_3$ starts to decrease, so that $C_3 < C$. In fact we observe from Eq.(11) that $C_3$ just saturates as a function of $\Delta$ for $\Delta \gtrsim 1.7$ and its value can already reasonably reproduce $C$. We stress again completely different behavior is for $\Delta < 1$ and $s = 0$. In this case one gets $C_3 = 0$ (as well as higher overlaps $C_{n>3} = 0$ due to particle-hole symmetry), hence the Mazur inequality with local conserved quantities is unable to reproduce $C > 0$ at $s = 0$ [5].

Let us further consider the normalized Drude weight $D^* = D/c_{\text{kin}}$, which represents the relative weight of the dissipationless transport within the whole sum rule, Eq.(8), i.e., we have $0 < D^* < 1$. Since one cannot perform a systematic extrapolation $L \rightarrow \infty$ for arbitrary magnetization $s$ we present in Fig. 6 results for $D^*$ within the whole (half) plane $\Delta, s \geq 0$ as calculated in systems with fixed $L = 19$. Apart from some anomalies observed (without the correction $\delta C$) already in Fig. 3 we confirm quite regular dependence $D^*(s)$ on $(\Delta, s)$. It is quite evident that in the limiting case $\Delta = 0$ (XY model) we get $D^* = 1$ corresponding to noninteracting fermions where the whole sum rule is within the Drude weight. The same hold for maximal magnetization $s \rightarrow \pm 1/2$ (for nearly empty or full band, $n \rightarrow 0, n \rightarrow 1$, respectively) where the interaction does not play a role. For fixed $\Delta$ the minimum of $D^*$ is always at $s = 0$ whereby the dependence $D^*(s)$ is nearly universal for all $\Delta > 1$.

B. Finite Temperature

Finally, let us present results for the $T$-dependence $D(T)$ as evaluated using the relation (6), again restricting our analysis to zero magnetization $s = 0$ and systems with odd $L$ (Fig. 7). It should be realized that numerical results at low $T < 0.5$ are more susceptible to finite-size effects since very small number of MB levels effectively participate in $D(T)$ and the crucial contribution comes from the ground state $\epsilon_0(\phi)$. Still, in spite of some discrepancies at low $T < 0.4$ the overall agreement with the TBA result [13] is reasonable. Another conclusion is that the extended high-$T$ behavior, i.e. $D = C/T$ is followed very accurately down to quite low $T > 0.5$ in the whole range.
Finite-\( T \) Drude weight \( D(T) \) for \( \Delta < 1 \) at magnetization \( s = 0 \) as calculated numerically using ED with \( L = 15 - 21 \) and finite-size scaling (full line with dots), extrapolating the high-\( T \) numerical result, i.e. \( D = C/T \) (thin lines), and Thermodynamic Bethe Ansatz result (dots) from Ref. [13].

\( \Delta < 1 \). While the ground state value \( D_0 \) is quite reliable in the intermediate window \( 0 < T < 0.5 \) results are sensitive to finite-size effects so we cannot give a firm conclusion on possible nonanalytical low-\( T \) behavior as predicted in Ref. [13].

\[ \delta C = T \Delta \] is very well reproduced from the TBA result [13], in this way possibly eliminating (or at least restricting) some recently expressed questions regarding its validity.

High-\( T \) normalized Drude weight \( D^* \) away from \( s = 0 \) shows a systematic and smooth variation with \( s \) towards the limiting values \( D^* = 1 \) for \( s = \pm 1/2 \) as well as in XY limit \( \Delta = 0 \). In the Ising regime \( \Delta > 1 \) (in particular for large \( \Delta > 2 \)) the variation \( C = TD(s) \) is very well reproduced with the Mazur inequality overlap with the conserved energy current \( j_E \), in very contrast to the XY-type regime \( \Delta < 1 \).

Results for the \( T \)-variation \( D(T) \) reveals that even quantitatively the high-\( T \) result \( D = C/T \) remains valid in a wide regime, i.e., generally for \( T > 0.5 \). While small-system results allow also for a reliable scaling for \( D_0 = D(T = 0) \) at \( s = 0 \), the finite-size effects are rather hard to avoid in the window \( 0 < T < 0.5 \) and other methods beyond the ED are needed to investigate in more detail this regime.

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IV. CONCLUSIONS

In conclusion, we have shown that numerical evaluation of the Drude weight (spin stiffness) \( D(T) \) within the anisotropic Heisenberg model can lead to more controlled and converged results if performed in a canonical ensemble, at fixed \( S_z \) (number of particles \( N \)). Breaking of the particle-hole symmetry by using systems with odd \( L \) is also helpful and is advantageous over usually studied systems with even \( L \). Our study is mostly concentrated on the high-\( T \) limit which should be anyhow quite generic for the whole regime \( T > 0 \). Results obtained at zero magnetization \( s = 0 \) using the finite-size scaling confirm the change of character of \( D(T) \) at \( \Delta = 1 \), i.e., they are compatible with the \( D(T) = 0 \) for \( \Delta > 1 \). While at \( s = 0 \) within the majority of the regime \( \Delta < 1 \) there are no evident problems with the scaling \( 1/L \) of \( D(T) \) we have traced the irregularities at \( \Delta < 0.5 \) back to the emergence of finite-size low-\( \omega \) contribution in \( \sigma_{reg}(\omega) \) which can lead to a finite correction \( \delta C \) in the thermodynamic limit \( L \to \infty \). Taken the latter into account, we find a very good agreement with the TBA result [13], in this way possibly eliminating (or at least restricting) some recently expressed questions regarding its validity.

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