Magnetic excitation spectra of strongly correlated quasi-one dimensional systems: Heisenberg versus Hubbard-like behavior

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I. HEISENBERG MODEL ON A CHAIN: COMPARISON WITH EXACT TWO-SPINON RESULTS

In this section, we compare the Krylov method with the exact two-spinon results obtained in ref. 1 for an antiferromagnetic Heisenberg chain. We focus on a particular cut at $k = \pi/2$ of the dynamical spin structure factor. The figure shows a good agreement between the analytical and numerical results. In the DMRG simulations, we increase the system size from $L = 64$ to $L = 128$ sites and reduce the broadening η from 0.05 to 0.025. Larger systems sizes and smaller broadenings η are needed to converge to the exact results.

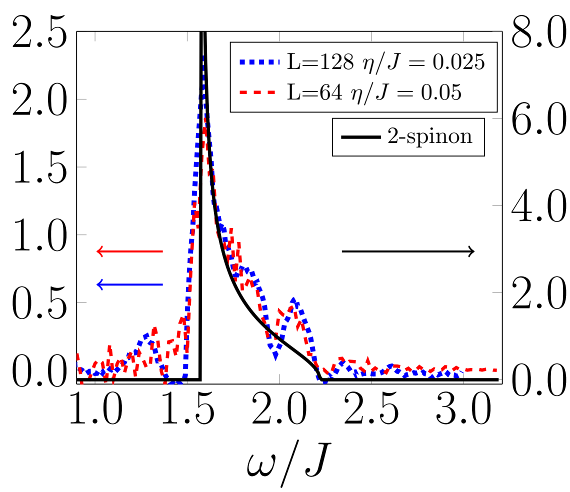

FIG. 1: (Color online) Cuts at $k = \pi/2$ for the spin dynamical structure factor for a Heisenberg chain. The 2-spinon exact results (solid black line) are calculated from expression in ref. 1. Data refers to the right y axis. The DMRG data (dotted and dashed lines) refer to the left y axis and are obtained on a chain of $L = 64$ and $L = 128$ sites, using $m = 1000$ states. The data in both vertical axes is in arbitrary units.

II. COMPARISON OF HUBBARD AND HEISENBERG MODELS USING LADDER GEOMETRIES

In this section, we complement the study of ladders reported in the main text by analyzing the cuts of the two branches of the magnetic excitation spectrum at the special case $k_x = \pi$.

As observed in fig.6 (a) of the main text, a spin gap is visible already for $U = 1$. This significantly affects the shape of the spectrum of the inter-band electronic spin excitations; see the dashed (red) curve in panel (a) of fig. 2. In fact, the magnetic spin excitations develop a pronounced (π, π) peak at $\omega/(4t) \simeq 0.01$ already for $U = 0.5$. Contrary to the inter-band spin excitations, the intra-band spin excitations are not much affected by the electronic correlations: the (red) dashed curve in panel (c) of fig. 2 shows just a shift to lower frequency, while the spectral shape feature is only slightly distorted.

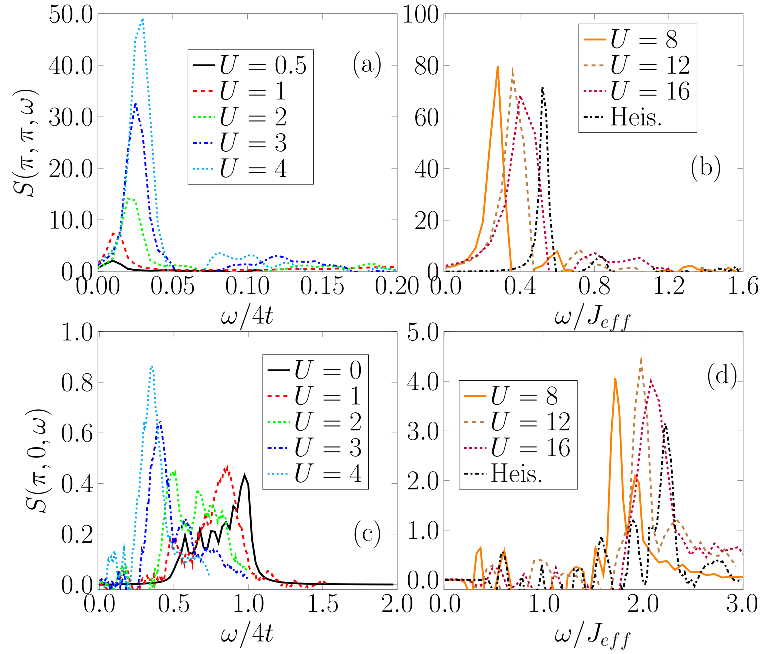

FIG. 2: (Color online) Cuts of the spin dynamical structure factors $S(\pi, \pi, \omega)$ (panels a and b) and $S(\pi, 0, \omega)$ (panels c and d) for a system with $L = 32 \times 2$ sites as a function of $\omega/(4t)$ (panel a and c) and $\omega/J_{\rm eff}$ (panel b and d), at different values of U. As in the chain case, we have assumed $J_{\rm eff} = 4t_y^2/U$. In the DMRG simulations, $\eta = 0.02t$ has been considered for the Hubbard model while $\eta = 0.02J$ for Heisenberg, with $\Delta\omega = 0.01$ and with up to $m = 1000$ DMRG states kept.

At $U = 2$, the $(\pi, 0)$ cut of the magnetic excitation spectrum starts to be significantly modified by the effect of the electronic correlations. The entire non-zero spectral features of intra-band excitations becomes further shifted to lower frequencies, while a double peak structure starts to appear as in the chain case. The high-energy peak resembles the non-interacting part of the excitation band, while the lower energy peak at $\omega/(4t) \simeq 0.5$ points toward Heisenberg-like behavior resembling the two-triplet bound state peak. In the (π, π) cut of the spectrum, an increase in the spin gap is visible, while the effects of the spectral redistribution point to a higher magnetic (π, π) peak.

For $U = 3$ and $U = 4$, the spectral weight redistribution to lower frequencies continues. In the $(\pi, 0)$ cut of the magnetic spectrum—the (blue) dashed-dotted and (cyan) dotted line in panel (c) of fig. 2— a well defined $(\pi, 0)$ peak appears at $\omega/(4t) \simeq 0.4$ for $U = 3$, and at $\omega/(4t) \simeq 0.35$ for $U = 4$. Yet the high-energy peak, characteristic of the non-interacting case, appears barely visible in the high-frequency tail around $\omega/(4t) \simeq 0.75$ for $U = 3$, while it disappears completely for $U = 4$. Recall that in the non-interacting case, this high-energy peak had of the same spectral weight as the lower peak in the $U = 2$ case.

In the $k_y = \pi$ portion of the spectrum, the same behavior as observed for the $U = 1$ case can be seen again for $U = 2$ and $U = 3$, and in general up to $U = 16$, the highest value of U we have investigated; see panel (a) and (b) of fig. 2. The spin gap increases together with the magnetic (π, π) peak height. The results are shown to *converge* to the spectrum obtained in the Heisenberg model case, once we plot them according to the ratio $\omega/J_{\rm eff}$. In panel (d) of fig. 2, the $k_y = 0$ cuts of the spectrum for $U > 4$ show similar convergence: the results get closer and closer to the Heisenberg model calculations with increasing U as expected.

III. SUPPLEMENTAL: REPRODUCING THE NUMERICAL RESULTS.

The DMRG++ code can be obtained with:

```
git clone https://github.com/g1257/dmrgpp.git
```

and PsimagLite with:

```
git clone https://github.com/g1257/PsimagLite.git
```

To compile:

```
cd PsimagLite/lib
perl configure.pl
(you may now optionally edit Config.make)
make
cd ../../dmrgpp/src
perl configure.pl
(you may now optionally edit Config.make)
make
```

To compute the spectrum shown in Figure 1, say panel c, corresponding to the dynamical spin structure factor of a Hubbard chain with $L = 64$ sites and $U = 2t$, first use the input file `input_L64_Hubbard_chain.inp` to calculate the ground state of the system:

```
TotalNumberOfSites=64
NumberOfTerms=1

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1  -1.0

Model=HubbardOneBand
hubbardU 64    2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
               2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
potentialV 128 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

SolverOptions=twositedmrg
Version=version
OutputFile=DataGS.txt
InfiniteLoopKeptStates=64
FiniteLoops 5
 31 1000 0 -62 1000 0
 62 1000 0 -62 1000 0
 62 1000 0

TargetElectronsUp=32
TargetElectronsDown=32
TruncationTolerance=1e-8
```

Above, a maximum of $m = 1000$ states are kept in the simulation by keeping the DMRG truncation error below 10^{-8}. One can run the code executing the command

```
./dmrg -f input_L64_Hubbard_chain.inp.
```

Once the ground state $|\Psi_0\rangle$ has been obtained, restart from ground state calculations. In order to calculate the dynamical structure factor in frequency space

$$S_{j,c}(\omega + i\eta) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\Psi_0|S^z_j \frac{1}{\omega - \hat{H} + E_0 + i\eta} S^z_c|\Psi_0\rangle\right], \tag{1}$$

restart from the ground state calculation with input `input_L64_Hubbard_x.inp` for each desired $\omega = x$ value of the spectrum:

```
TotalNumberOfSites=64
NumberOfTerms=1

DegreesOfFreedom=1
```

```
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1  -1.0

Model=HubbardOneBand
hubbardU 64    2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
               2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
potentialV 128 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

InfiniteLoopKeptStates=64
FiniteLoops 3
-62 1000 2 62 1000 2 -62 1000 2

SolverOptions=CorrectionVectorTargetting,restart,twositedmrg
CorrectionA=0
Version=version

TruncationTolerance=1e-8

OutputFile=datax.txt

DynamicDmrgType=0
TSPSites 1 31
TSPLoops 1 1
TSPProductOrSum=sum
CorrectionVectorFreqType=Real

CorrectionVectorEta=0.05
CorrectionVectorAlgorithm=Krylov
TridiagEps=1e-7
TridiagSteps=1000

RestartFilename=DataGS.txt

GsWeight=0.1
CorrectionVectorOmega=x

TSPOperator=raw
RAW_MATRIX
4 4
0 0 0 0
0 0.5 0 0
0 0 -0.5 0
0 0 0 0
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

Notice the `restart` and `CorrectionVectorTargetting` flags in the `SolverOptions` of the code. In eq. 1, $\hat{H}$ and E_0 represent the Hamiltonian and the ground state energy of the Hubbard model. User must substitute x with the value of desired value ω. This input restarts the DMRG simulations applying to the ground state $|\Psi_0\rangle$ the operator S^z_c, represented explicitly at the bottom of the input as

```
TSPOperator=raw
RAW_MATRIX
4 4
```

```
0 0 0 0
0 0.5 0 0
0 0 -0.5 0
0 0 0 0
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

at the center of the chain $c = L/2 - 1 = 31$ using the flag `TSPSites 1 31`. The code calculates then the correction vector

$$|x(\omega + i\eta)\rangle \equiv \frac{1}{\omega - \hat{H} + E_0 + i\eta} S^z_c |\Psi_0\rangle \tag{2}$$

for each frequency $\omega = x$ and $\eta = 0.05$. The expression in eq. 1 is calculated as

$$S_{j,c}(\omega + i\eta) = -\frac{1}{\pi}\text{Im}\Bigg[\langle\Psi_0|S^z_j|x(\omega + i\eta)\rangle\Bigg] \tag{3}$$

with

```
./dmrg -f input_L64_Hubbard_x.inp 'z',
```

where the option `'z'` means that we are measuring *in situ* the spin operator S^z_j on all the sites of the chain. In the output file `runForinputx.cout`, they are going to appear lines such as

```
j re 0 <PSI|z|P2> <PSI|P2>
..
j im 0 <PSI|z|P3> <PSI|P3>
```

where `|P2>` and `|P3>` represent the real and imaginary part of the correction vector $|x(\omega + i\eta)\rangle$, `|PSI>` the ground state, while `re` and `im` the real and imaginary part of the correlator $\langle\Psi_0|S^z_j|x(\omega + i\eta)\rangle$. Collecting the data for all sites j allows us to calculate the $S(k, \omega)$ in frequency momentum space.

Above, the correction vector is calculated with the Krylov method presented in the main text; notice the lines

```
CorrectionVectorAlgorithm=Krylov
TridiagEps=1e-7
TridiagSteps=1000
```

where a maximum of 1000 iteration steps is set keeping the Lanczos error below 10^{-7}. The Krylov method for the computation of the correction vector has been discussed in ref. 2. We finally provide the input for computing the ground state for a Hubbard ladder `input_L64_Hubbard_ladder.inp` with $L = 48 \times 2$ site at half-filling and $t_x = t_y = t$ and interaction strength $U = 16t$

```
TotalNumberOfSites=96
NumberOfTerms=1

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors   1  -1.0
Connectors   1  -1.0
LadderLeg=2

Model=HubbardOneBand
hubbardU 96    16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
               16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
               16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
               16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
               16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
               16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
```

```
potentialV 192 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

SolverOptions=twositedmrg
Version=version
OutputFile=DataGS.txt
InfiniteLoopKeptStates=64
FiniteLoops 5
 47 1000 0 -94 1000 0
 94 1000 0 -94 1000 0
 94 1000 0

TargetElectronsUp=48
TargetElectronsDown=48
TruncationTolerance=1e-8
```

The dynamical spin structure factor for this system was shown in panels (a) (b) of Fig. 5 and can be obtained similarly along the same lines explained above. Other inputs for the Heisenberg model case are discussed in the supplemental material of ref. 2.

---

[1] M. Karbach, G. Müller, A. H. Bougourzi, A. Fledderjohann, and K.-H. Mütter, Phys. Rev. B **55**, 12510 (1997), URL http://link.aps.org/doi/10.1103/PhysRevB.55.12510.

[2] A. Nocera and G. Alvarez, arXiv preprint arXiv:1607.03538 (2016).