Supplementary Materials for "Multi-spinon and antiholon excitations probed by resonant inelastic x-ray scattering on doped one-dimensional antiferromagnets"

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I. REPRODUCING THE DMRG 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
```

For the numerical results shown in the main text, PsimagLite version 2.02 and DMRG++ version 5.03 were used. Below, we will describe the input files needed to reproduce the $S(q,\omega)$ and $N(q,\omega)$ data in Fig. 3 of the main text. For convenience, we include the ground state input file, `inputGS.inp`, valid for a *doped* t-J chain with a system size $L = 8$, using only $m = 100$ DMRG states.

```
TotalNumberOfSites=8
NumberOfTerms=4

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.3

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.0625
```

```
Model=TjMultiOrb

potentialV 16
0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0

InfiniteLoopKeptStates=100
FiniteLoops 5
 3 100 0
-6 100 0 6 100 0
-6 100 0 6 100 0

TargetElectronsUp=3
TargetElectronsDown=3
Threads=1
SolverOptions=twositedmrg,useSvd
TruncationTolerance=1e-6
Version=version
OutputFile=dataGS.txt
Orbitals=1
```

This input could be executed quickly on a standard laptop as

```
./dmrg -f inputGS.inp
```

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

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

restart from the ground state calculation with input `input_275.inp` for each desired, say $\omega = 0.275$, value of the spectrum:

```
TotalNumberOfSites=8
NumberOfTerms=4

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.3

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.0625

Model=TjMultiOrb

potentialV 16
```

```
0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0

InfiniteLoopKeptStates=100
FiniteLoops 3
-6 100 2 6 100 2 -6 100 2

TargetElectronsUp=3
TargetElectronsDown=3
TruncationTolerance=1e-6
SolverOptions=CorrectionVectorTargetting,twositedmrg,restart,useSvd,minimizeDisk
CorrectionA=0
Version=version
RestartFilename=dataGS.txt

OutputFile=data275.txt

DynamicDmrgType=0
TSPSites 1 3
TSPLoops 1 1
TSPProductOrSum=sum
CorrectionVectorFreqType=Real

CorrectionVectorEta=0.08
CorrectionVectorAlgorithm=Krylov
TridiagEps=1e-8
TridiagSteps=200
Orbitals=1

GsWeight=0.1
CorrectionVectorOmega=0.275

TSPOperator=raw
RAW_MATRIX
3 3
0 0 0
0 0.5 0
0 0 -0.5
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 t-J model on a chain. 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
3 3
0 0 0
0 0.5 0
0 0 -0.5
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

at the center of the chain $c = L/2 - 1 = 3$ using the flag `TSPSites 1 3`. 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 the frequency $\omega = 0.275$ and $\eta = 0.08$. The expression in eq. 1 is calculated as

$$S_{j,c}(\omega + i\eta) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\Psi_0|S_j^z|x(\omega + i\eta)\rangle\right] \tag{3}$$

with

```
./dmrg -f input_275.inp 'z',
```

where the option `'z'` means that we are measuring *in situ* the spin operator S_j^z on all the sites of the chain. In the output file `runForinput_275.cout`, they are going to appear lines such as

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

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

The reader can modify the input given above to compute the dynamical spin structure factor $S(q, \omega)$ for a longer $L = 80$ sites chain.

The Krylov method for the computation of the correction vector has been discussed in ref. 1 and computational details are provided in its supplemental material; Notice the lines

```
CorrectionVectorAlgorithm=Krylov
TridiagEps=1e-8
TridiagSteps=200
```

where a maximum of 200 iteration steps is set keeping the Lanczos error below 10^{-6}.

In order to calculate the dynamical charge structure factor in frequency space

$$N_{j,c}(\omega + i\eta) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\Psi_0|(n_j - \langle n_j\rangle)\frac{1}{\omega - \hat{H} + E_0 + i\eta}(n_c - \langle n_c\rangle)|\Psi_0\rangle\right], \tag{4}$$

one needs to first compute the local densities $\langle n_j\rangle$ in the ground state as

```
./observe -f inputGS.inp '<gs|n|gs>'.
```

Then, one needs to produce files `nx.txt` for each site `x` of the chain, including the fluctuation operators matrices $(n_j - \langle n_j\rangle)$. The local occupation operator is given by

```
TSPOperator=raw
RAW_MATRIX
3 3
0 0 0
0 1 0
0 0 1
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

With the above input parameters, for the center site of the chain we have $\langle n_c\rangle = 0.738889$. Therefore, the fluctuation operator matrix is

```
TSPOperator=raw
RAW_MATRIX
3 3
-0.738889 0 0
0 0.261111 0
0 0 0.261111
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

and needs to be stored in a file `n3.txt`. Finally, the input file `inputN_275.inp` to compute the dynamical charge correlation function at frequency $\omega = 0.275$ is

```
TotalNumberOfSites=8
NumberOfTerms=4

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.3

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 0.25

DegreesOfFreedom=1
GeometryKind=chain
GeometryOptions=ConstantValues
Connectors 1 -0.0625

Model=TjMultiOrb

potentialV 16
0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0

InfiniteLoopKeptStates=100
FiniteLoops 3
-6 100 2 6 100 2 -6 100 2

TargetElectronsUp=3
TargetElectronsDown=3
TruncationTolerance=1e-6
SolverOptions=CorrectionVectorTargetting,twositedmrg,restart,useSvd,minimizeDisk
CorrectionA=0
Version=version
RestartFilename=dataGS.txt

OutputFile=data275.txt

DynamicDmrgType=0
TSPSites 1 3
TSPLoops 1 1
TSPProductOrSum=sum
CorrectionVectorFreqType=Real

CorrectionVectorEta=0.025
CorrectionVectorAlgorithm=Krylov
TridiagEps=1e-7
TridiagSteps=1000
Orbitals=1

GsWeight=0.1
```

```
CorrectionVectorOmega=0.275

TSPOperator=raw
RAW_MATRIX
3 3
-0.738889 0 0
0 0.261111 0
0 0 0.261111
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

The code above calculates then the correction vector

$$|w(\omega + i\eta)\rangle \equiv \frac{1}{\omega - \hat{H} + E_0 + i\eta}(n_c - \langle n_c \rangle)|\Psi_0\rangle. \tag{5}$$

The expression in eq. (4) is then calculated as

$$N_{j,c}(\omega + i\eta) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\Psi_0|(n_j - \langle n_j\rangle)|w(\omega + i\eta)\rangle\right] \tag{6}$$

with

`./dmrg -f inputN_275.inp 'n$.txt',`

where the option `'n$.txt'` means that we are measuring *in situ* the charge operators $n_j - \langle n_j \rangle$ on all the sites of the ladder. In the output file `runForinput_275.cout`, they are going to appear lines such as

```
j im 0 <PSI|n$.txt|P2> <PSI|P2>
..
j re 0 <PSI|n$.txt|P3> <PSI|P3>
```

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

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[1] A. Nocera and G. Alvarez, Phys. Rev. E **94**, 053308 (2016), URL https://link.aps.org/doi/10.1103/PhysRevE.94.053308.