Signatures of pairing in the magnetic excitation spectrum of strongly correlated two-leg ladders

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I. PAIRING STRENGTH FROM GROUND STATE CORRELATIONS.

In this section, we study the dependence of the ground state pairing strength $\bar{D}$ defined as $\bar{D} = \sum_{i=l}^{u} P(i)/P(1)$ on the lower l and upper u limits in the sum. We have verified that the results shown in the main text do not change

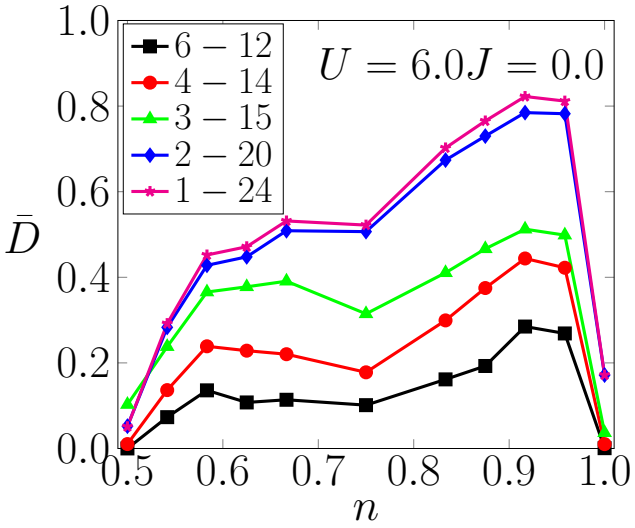

FIG. 1: (Color online) Pairing correlation strength $\bar{D}$ as a function of doping n for a ladder with $U = 6.0$ and $J = 0.0$. Different lower and upper limits have been used (l,u)= $\{(6-12), (4-14), (3-15), (2-20), (1-24)\}$.

qualitatively modifying these limits: choosing 6, as opposed to e.g. 1, reduces artificial short-distance effects while 12, as opposed to e.g. 24, reduces edge effects. Short-distance and edge effects are however not severe. Fig.1 shows the pairing strength as a function of doping for a ladder with $U = 6.0$ and $J = 0.0$ using different limits in the definition of $\bar{D}$.

II. 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 ground state properties of the t-U-J ladder studied in the main text, consider the following input file `input.inp`:

```
TotalNumberOfSites=96
NumberOfTerms=5

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

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  -0.125
Connectors 1  -0.125
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0
Connectors 1  0
LadderLeg=2

Model=HubbardOneBandExtendedSuper

hubbardU 96 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6

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

InfiniteLoopKeptStates=128
FiniteLoops 7
47 1000 0
-94 1000 0 94 1000 0
-94 1000 0 94 1000 0
-94 1000 0 94 1000 1

TargetElectronsUp=42
TargetElectronsDown=42
Threads=24
SolverOptions=twositedmrg,useSvd,MatrixVectorKron
Version=version
TruncationTolerance=1e-7
LanczosEps=1e-7
OutputFile=dataGS.txt
Orbitals=1
```

Above, a maximum of $m = 1000$ states are kept in the simulation by keeping the DMRG truncation error below 10^{-7}. We have furthermore considered $U = 6.0$, $J = 0.5$ and doping $n = 0.875$. We notice that computer cluster resources are needed for the production runs. For this reason we include below an input file, `input_L8x2.inp`, valid for a shorter system size $L = 8 \times 2$, using only $m = 200$ DMRG states. `input_L8x2.inp` could be executed quickly on a standard laptop.

```
TotalNumberOfSites=16
NumberOfTerms=5

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

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  -0.125
Connectors 1  -0.125
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2
```

```
DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0
Connectors 1  0
LadderLeg=2

Model=HubbardOneBandExtendedSuper

hubbardU 16
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6

potentialV 32
0 0 0 0 0 0 0 0 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=128
FiniteLoops 5
7 200 0
-14 200 0 14 200 0
-14 200 0 14 200 1

TargetElectronsUp=7
TargetElectronsDown=7
SolverOptions=twositedmrg,useSvd,MatrixVectorKron
Version=version
TruncationTolerance=1e-7
LanczosEps=1e-7
OutputFile=dataGS.txt
Orbitals=1
```

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

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

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

```
TotalNumberOfSites=96
NumberOfTerms=5

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

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  -0.125
Connectors 1  -0.125
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
```

```
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0.5
Connectors 1  0.5
LadderLeg=2

DegreesOfFreedom=1
GeometryKind=ladder
GeometryOptions=ConstantValues
Connectors 1  0
Connectors 1  0
LadderLeg=2

Model=HubbardOneBandExtendedSuper

hubbardU 96 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6

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

InfiniteLoopKeptStates=128
FiniteLoops 3
-94 1000 2 94 1000 2 -94 1000 2

TargetElectronsUp=42
TargetElectronsDown=42

SolverOptions=CorrectionVectorTargetting,twositedmrg,restart,useSvd,MatrixVectorKron,minimizeDisk
CorrectionA=0
Version=version
Threads=24
RestartFilename=dataGS.txt
TruncationTolerance=1e-7
LanczosEps=1e-7

OutputFile=data275.txt

DynamicDmrgType=0
TSPSites 1 46
TSPLoops 1 1
TSPProductOrSum=sum
CorrectionVectorFreqType=Real
```

```
CorrectionVectorEta=0.08
CorrectionVectorAlgorithm=Krylov
TridiagonalEps=1e-7
TridiagSteps=1000
Orbitals=1

GsWeight=0.1
CorrectionVectorOmega=0.275

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 t-U-J model. 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 ladder $c = L/2 - 2 = 46$ using the flag `TSPSites 1 46`. 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

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

with

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

where the option `'z'` means that we are measuring *in situ* the spin operator S^z_j 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 $\langle \Psi_0 | S^z_j | x(\omega + i\eta) \rangle$. Collecting the data for all sites j allows us to calculate the $S(k, \omega)$ in frequency momentum space.

The reader can modify the input given above to compute the dynamical spin structure factor $S(k, \omega)$ for a shorter $L = 8 \times 2$ ladder.

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-7
TridiagSteps=1000
```

where a maximum of 1000 iteration steps is set keeping the Lanczos error below 10^{-7}.

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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.