Symmetry Conserving Purification of Quantum States within the Density Matrix Renormalization Group

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I. 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 dmrgpp/src
perl configure.pl
(all defaults)
make
```

To obtain the square curve of Figure 1, which correspond to the Grand Canonical purification scheme for a Heisenberg chain with $L = 6$ sites, first use `Fig1_DMRG_GC_L6_entangler.inp` as input to generate the infinite temperature state

```
./dmrg -f Fig1_DMRG_GC_L6_entangler.inp &> out_entangler_GC.
```

The ground state energy of the entangler Hamiltonian can be monitored with

```
grep Energy dataGS.txt.
```

Second, restart with this result using `Fig1_DMRG_GC_L6.inp` as input to evolve in imaginary time

```
./dmrg -f Fig1_DMRG_GC_L6.inp &> out_GC.
```

The local energies at temperature T can be obtained with a *Perl* script `getEnergy.pl`

```
perl getEnergy.pl betaprime time < out_GC,
```

where `betaprime` should be substituted by the actual numerical value $\beta' = \beta/2 = 1/2T$. To obtain the circle curve of Figure 1, corresponding to the Canonical purification scheme, first use `Fig1_DMRG_C_L6_entangler.inp` as input to generate the the infinite temperature state; then, restart with this result using `Fig1_DMRG_C_L6.inp` as input to evolve in imaginary time.

The input files for generating Figure 2 of the manscript can be obtained by generalizing the inputs discussed above.

Using the same procedure outlined for the Heisenberg model, in order to obtain the curves of Figure 3 corresponding to canonical scheme $C1$ and $C2$ for a $L = 6$ sites t-J model, first use

```
Fig3_DMRG_C1_L6_entangler.inp,
Fig3_DMRG_C2_L6_entangler.inp
```

to generate the maximally entangled temperature states for the $C1$ and $C2$ Canonical purification, respectively. Then, restart the result obtained using

```
Fig3_DMRG_C1_L6.inp,
Fig3_DMRG_C2_L6.inp,
```

as inputs to evolve in imaginary time.

Finally, we provide the input file for generating the infinite temperature maximally entangled state of type C2 for a $L = 6$ sites chain Hubbard model

```
Fig4_DMRG_C2_L6_entangler.inp.
```

One can obtain the (dark green) empty circles curve in the inset of Figure 4 by evolving

```
./dmrg -f Fig4_DMRG_C2_L6.inp &> out_C2.
```

The scaling analysis performed in the main panel of Figure 4 can be obtained by generalizing the inputs provided above.

II. PROOF OF OBSERVATION (3) IN APPENDIX A

Observation 1. *For any Hamiltonian with convex energies and an extensive canonical partition function, at finite temperature, and in the thermodynamic limit, the average energy in the canonical ensemble is the same as the one in the grand canonical ensemble.*

Proof. Let M be the number of sites, considering spin and orbitals, such that the maximum number of electrons that the system can hold is M. Let n_T be the target density of electrons, and let μ_M be such that $\langle N\rangle_{\mathrm{GC}}/M = n_T$. Let $Z_{C,M,N}(\beta)$ be the canonical partition function for N electrons and $Z_{GC,M,\mu_M}(\beta)$ the grand canonical one at μ_M. Because the canonical partition function is extensive, in the thermodynamic limit we have $Z_{C,M,N}(\beta) = z_{C,n}^M$, where $n = N/M$.

$$\lim_{M\to\infty} Z_{GC,M,\mu_M}(\beta) = \lim_{M\to\infty} \sum_{n=0}^{1} \left(z_{C,n} \exp(\beta\mu_M n)\right)^M \tag{1}$$

Moreover, $z_{C,n}$ has a maximum at $n = n_T$, and because the energies are convex this maximum is unique. In the thermodynamic limit then

$$\lim_{M\to\infty} Z_{GC,M,\mu_M}(\beta) = \lim_{M\to\infty} \left(z_{C,n_T} \exp(\beta\mu_M n_T)\right)^M, \tag{2}$$

which, up to a constant, is equal to the canonical partition function z_{C,n_T}^M. □