Exact Values of Internal Energy and Specific Heat of Finite Lattices

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The following (short) documentation is about the computation of the exact values of the internal energy and the specific heat of finite lattices. The according implementation realizes the method given in [1].

The starting point is the canonical partition function $Z_{mn}(T)$ of a $m \times n$ square Ising lattice wrapped on a torus and in zero magnetic field

$$Z_{mn}(T) = \frac{1}{2}(2\sinh(2K))^{\frac{1}{2}mn} \sum_{i=1}^{4} Z_i(K)\,, \quad K = \frac{J}{k_{\mathrm{B}}T}\,, \tag{1}$$

whereas $J_x = J_y = J$ and the Z_i are the partial partition functions

$$\begin{aligned} Z_1 &= \prod_{r=0}^{n-1} 2\cosh\left(\frac{1}{2}m\gamma_{2r+1}\right)\,, & Z_2 &= \prod_{r=0}^{n-1} 2\sinh\left(\frac{1}{2}m\gamma_{2r+1}\right)\,, \\ Z_3 &= \prod_{r=0}^{n-1} 2\cosh\left(\frac{1}{2}m\gamma_{2r}\right)\,, & Z_4 &= \prod_{r=0}^{n-1} 2\sinh\left(\frac{1}{2}m\gamma_{2r}\right)\,. \end{aligned} \tag{2}$$

The internal energy per site is given by

$$\begin{aligned} \frac{U_{mn}}{mn} &= -\frac{J}{mn}\frac{\mathrm{d}}{\mathrm{d}K}\ln Z_{mn} \\ &= -J\coth(2K) - \frac{J}{mn}\left[\sum_{i=1}^{4} Z_i'\right]\left[\sum_{i=1}^{4} Z_i\right]^{-1}\,, \end{aligned} \tag{3}$$

while the specific heat per site is

$$\begin{aligned} \frac{C_{mn}}{k_{\mathrm{B}}mn} &= \frac{K^2}{mn}\frac{\mathrm{d}^2}{\mathrm{d}K^2}\ln Z_{mn} \\ &= -2K^2\csc^2(K) + \frac{K^2}{mn}\left[\frac{\sum_{i=1}^{4} Z_i''}{\sum_{i=1}^{4} Z_i} - \left(\frac{\sum_{i=1}^{4} Z_i'}{\sum_{i=1}^{4} Z_i}\right)^2\right]\,. \end{aligned} \tag{4}$$

The primes denote the differentiation with respect to K.

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To evaluate the partial partition functions and their derivatives, the following expressions will be required:

$$
\begin{aligned}
\gamma_0 &= 2K + \ln(\tanh(K))\,, \\
\gamma_{r\neq 0} &= \ln(c_r + (c_r^2 - 1)^{1/2})\,, \\
c_r &= \cosh(2K)\coth(2K) - \cos(r\pi/n)\,,
\end{aligned}
$$

$$
\begin{aligned}
\gamma_0' &= 2(1 + \csc(2K))\,, \\
\gamma_{r\neq 0}' &= c_r'(c_r^2 - 1)^{-1/2}\,, \\
c_r' &= 2\cosh(2K)(1 - \csc^2(2K))\,,
\end{aligned}
$$

$$
\begin{aligned}
\gamma_0'' &= -4\csc(2K)\coth(2K)\,, \\
\gamma_{r\neq 0}'' &= c_r''(c_r^2 - 1)^{-1/2} - (c_r')^2 c_r (c_r^2 - 1)^{-3/2}\,, \\
c_r'' &= 8\csc^3(2K)\cosh^2(2K) + 4(\sinh(2K) - \csc(2K))\,,
\end{aligned}
$$

$$
\begin{aligned}
Z_1'/Z_1 &= \frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\tanh(\tfrac{1}{2}m\gamma_{2r+1})\,, \\
Z_2'/Z_2 &= \frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\coth(\tfrac{1}{2}m\gamma_{2r+1})\,, \\
Z_3'/Z_3 &= \frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r}'\tanh(\tfrac{1}{2}m\gamma_{2r})\,, \\
Z_4'/Z_4 &= \frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r}'\coth(\tfrac{1}{2}m\gamma_{2r})\,,
\end{aligned}
$$

$$
\begin{aligned}
Z_1''/Z_1 &= \left[\frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\tanh(\tfrac{1}{2}m\gamma_{2r+1})\right]^2 \\
&\quad + \frac{1}{2}m\sum_{r=0}^{n-1}[\gamma_{2r+1}''\tanh(\tfrac{1}{2}m\gamma_{2r+1}) + \tfrac{1}{2}m(\gamma_{2r+1}'\mathrm{sec}(\tfrac{1}{2}m\gamma_{2r+1}))^2]\,, \\
Z_2''/Z_2 &= \left[\frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\coth(\tfrac{1}{2}m\gamma_{2r+1})\right]^2 \\
&\quad + \frac{1}{2}m\sum_{r=0}^{n-1}[\gamma_{2r+1}''\coth(\tfrac{1}{2}m\gamma_{2r+1}) - \tfrac{1}{2}m(\gamma_{2r+1}'\mathrm{csc}(\tfrac{1}{2}m\gamma_{2r+1}))^2]\,, \\
Z_3''/Z_3 &= \left[\frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r}'\tanh(\tfrac{1}{2}m\gamma_{2r})\right]^2 \\
&\quad + \frac{1}{2}m\sum_{r=0}^{n-1}[\gamma_{2r}''\tanh(\tfrac{1}{2}m\gamma_{2r}) + \tfrac{1}{2}m(\gamma_{2r}'\mathrm{sec}(\tfrac{1}{2}m\gamma_{2r}))^2]\,, \\
Z_4''/Z_4 &= \left[\frac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r}'\coth(\tfrac{1}{2}m\gamma_{2r})\right]^2 \\
&\quad + \frac{1}{2}m\sum_{r=0}^{n-1}[\gamma_{2r}''\coth(\tfrac{1}{2}m\gamma_{2r}) - \tfrac{1}{2}m(\gamma_{2r}'\mathrm{csc}(\tfrac{1}{2}m\gamma_{2r}))^2]\,.
\end{aligned}
$$

A possible implementation of (3) and (4) can be found in

```
FF_internalEnergy_specificHeat_mpfr.c
FF_internalEnergy_specificHeat.c
```

whereas the latter uses (`long double`) data types and therefor restricts the lattice size to (128×128) or asymmetric lattice with less then (128^2) lattices sites. This is due to the rapidly increasing partial partition functions (2).

The former one uses the GNU MPFR library for multiple-precision floating-point computations—if you want to use it, you will need to install the MPFR library on your system—and thus does not restrict the lattice size any longer.

The source files can be compiled as follows

```
gcc -O3 -lm FF_internalEnergy_specificHeat.c
gcc -O3 -lm -lgmp -lmpfr FF_internalEnergy_specificHeat_mpfr.c
```

When using the Intel-C-Compiler `icc` make sure that `remark #981` is disabled (`-wd981`), since there will be a lot of remarks due to operands that will be evaluated in unspecified order.

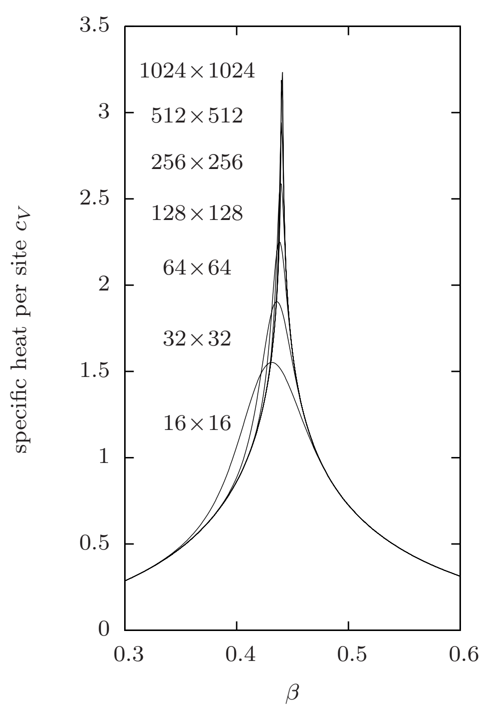
To use the program, open a terminal an type in the following line:

```
./FF_internalEnergy_specificHeat.x <K> <m> <n>
```

or similar for `FF_internalEnergy_specificHeat_mpfr.c`. The output will be of the form

```
<K> <internalEnergy> <specificHeat>.
```

The following plot shows the output of `FF_internalEnergy_specificHeat_mpfr.x` for different values of K an different lattice sizes.



References

[1] Arthur E. Ferdinand, Michael E. Fisher—Bounded and Inhomogeneous Ising Models. I. Specific-Heat Anomaly of a Finite Lattice; Phys. Rev. 185, 832 - 846 (1969)