We present simulation results for the thermodynamical behavior of flexible polymers (interacting self-avoiding walks) on simple-cubic (sc) and face-centered cubic (fcc) lattices. Besides the well-known collapse transition, we concentrate ourselves on the freezing transition occurring at lower temperatures.

We show how this transition, also called crystallization, liquid-solid [1] or globule-groundstate transition [2], is influenced by the lattice and how the transition depends on the system size.

We employ the pruned-enriched Rosenbluth method (PERM) [3] and generalized extensions of it [4,5].

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We will first concentrate on the low temperature region. To find some regularities anyhow in that region, we plot just all peak positions (Figure 3) and rearrange them, e.g. we plot the peak temperatures depending on polymer length (Figure 4).

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We see in Figure 8 a similar behavior to that in Figure 4. But the saw tooth behavior is not that clear anymore and the interpretation of the fluctuation is more complex. We found, for example, no ground-state with an energy gap, like the compact ones on the sc lattice.

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We investigate conformal transitions we concentrate on peaks (maxima) in the heat capacities. Figures 1 and 2 show heat capacities of short polymers on the sc lattice.

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What we see at low temperatures (T<1) are one or two maxima per chain length. There seems to be no consistent behavior depending on chain length. At high temperatures (T>1) we see the well known $\Theta$-Transition.

See Figure 5 for some visualizations of typical conformations.

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Looking at the freezing transition, we see that:
- there are periodical fluctuations of the transition temperature depending on polymer length ("saw tooth like", cp. Fig. 4);
- within these fluctuations the transition temperature remains constant.

Analyzing the fluctuations, we find:
- the jumps in transition temperature occur in vicinity of polymers, whose ground-states fill a cube or a rectangle (i.e. which have compact ground-states);
- these polymers have the "magic" lengths $N_{\text{sc}}=27, 36, 48, 64, 80$ and so on.

Figure 6 shows energy distribution around the freezing transition for the polymer with $N_{\text{sc}}=64$. Figure 7 visualizes corresponding conformations.

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Fitting the finite transition temperatures to following formula (suggested by Flory-Huggins theory, similar as in [1])

$$
\frac{1}{T(n)} = \frac{1}{T_0} + \frac{a_1}{N^{\frac{1}{2}}} + \frac{a_2}{N^{\frac{3}{4}}}
$$

we get:
- for sc: $T_0 = 3.717\pm0.007$ ($\alpha_1=2.5, \alpha_2=8.0$) (in perfect agreement to, e.g., Ref. [3])
- for fcc: $T_0=8.18\pm0.02$ ($\alpha_1=1.0, \alpha_2=5.5$)

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Freezing transition exists on sc and fcc lattice
- It is strongly influenced by lattice restrictions
- $\Theta$-transition peak becomes dominant
- Infinite $\Theta$-temperature could be reproduced (sc) and obtained (fcc)
- Both, $\Theta$ and freezing transition will not coincide in thermodynamic limit

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The $\Theta$-Transition Revisited

With presented method, it is possible to study reliably the freezing transition up to system sizes of order $10^4$. But there are no principal difficulties to study the $\Theta$-transition at higher temperatures up to lengths of order $10^3$ and with the original PERM algorithm up to order $10^5$ (at local temperatures). Results of the $\Theta$-temperature scaling are shown in Figure 10.