Exactly Soluble Models for Surface Partition

K. A. Bugaev[1,2], J. B. Elliott[1], L. Phair[1] and L. G. Moretto[1]
[1] *Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720*
[2] *Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine*

Within the frame work of recently suggested Hills and Dales Model (HDM) [1] we analyzed three partitions of surface deformations [2]. The HDM allows us to prove rigorously that the surface entropy of large clusters is proportional to the surface S, i.e. ωS (in dimensionless units), and obtain the upper and lower estimates for the coefficient ω, which is a ratio of the surface energy coefficient $\sigma_{\rm o}(T_c)$ per one constituent and the critical temperature T_c.

The main idea of the HDM is to account for all surface deformations of large cluster which have positive (hills) and negative (dales) heights. It is assumed that deformations are weighted by the Boltzmann factor of the surface energy cost $\exp\left(-\sigma_{\rm o}|\Delta S_k|/s_1/T\right)$ due to the change of the surface $|\Delta S_k|$ in units of the surface per constituent s_1. In addition, the surface deformations should conserve the volume of the cluster.

The grand canonical surface partition (GCSP), which was exactly solved earlier [1], obeys the volume conservation on average. Here we consider the canonical formalism for the HDM and obtain the infimum for the surface entropy of finite and large clusters. For the limit of vanishing deformations we also introduce the *semi-grand canonical ensemble* which occupies an intermediate place between the grand canonical and canonical surface ensembles. The Laplace-Fourier transform technique [3] allows us to evaluate exactly the canonical surface partition (CSP) and the semi-canonical surface partition (SGCSP) for any volume of the cluster.

In the limit of the vanishing amplitude of deformations we also found the upper $\max\{\omega^\alpha\}$ and lower $\min\{\omega^\alpha\}$ estimates for the ω-coefficient of large clusters for the GCSP ($\alpha = gc$), CSP ($\alpha = c$) and SGCSP ($\alpha = sgc$), which are given in Table I. The lower estimate corresponds to the smallest deformations.

Partition	$\max\{\omega^\alpha\}$	$\min\{\omega^\alpha\}$
GCSP	1.060090	0.852606
SGCSP	0.806466	0.567143
CSP	0.403233	0.283572

Table I. The maximal and minimal values of the ω-coefficient for three statistical partitions of the HDM.

These results are compared with the ω-coefficients for the large spin clusters of various 2- and 3-dimensional Ising model lattices, which are listed in the Tables II and III, respectively [4]. The ω-coefficient for the d-dimensional Ising model is defined as the energy $2J$ required to flip a given spin interacting with its q-neighbors to opposite direction per $(d-1)$-dimensional surface divided by the value of critical temperature

$$\omega_{Lat} = \frac{q\;J}{T_c\,d}\,. \tag{1}$$

Here q is the coordination number for the lattice, and J denotes the coupling constant of the model. A comparison of the Tables I - III shows that all lattice ω_{Lat}-coefficients, indeed, lie between the upper estimates for canonical and grand canonical surface partitions

$$0.40323 = \max\{\omega^c\} < \omega_{Lat} < \max\{\omega^{gc}\} = 1.06009. \tag{2}$$

Thus, we showed that $\max\{\omega^c\}$ and $\max\{\omega^{gc}\}$ are the infimum and supremum for 2- and 3-dimensional Ising models, respectively.

Lattice type	$\omega_{Lat} = \frac{\sigma}{T_c}$
Honeycomb	0.987718
Kagome	0.933132
Square	0.881374
Triangular	0.823960
Diamond	0.739640

Table II. The values of the ω_{Lat}-coefficient for various 2-dimensional Ising models. For more details see the text.

Lattice type	$\omega_{Lat} = \frac{\sigma}{T_c}$
Simple cubic	0.44342
Body-centered cubic	0.41989
Face-centered cubic	0.40840

Table III. The values of the ω_{Lat}-coefficient for various 3-dimensional Ising models.

[1] K. A. Bugaev, L. Phair and J. B. Elliott, nucl-th/0406034.
[2] K. A. Bugaev and J.B. Elliott, nucl-th/0501080.
[3] K. A. Bugaev, arXiv:nucl-th/0406033.
[4] M. E. Fisher, Rep. Prog. Phys. **30** (1969) 615.