

Phase Transition in Tensionless Surfaces

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Zaragoza, February 2004.

Overview of the talk

1. Some properties of surfaces
2. The continuum model
3. The discrete model
4. Some examples (MBE, liquid membranes, two dimensional melting)
5. Analytical calculations (variational approach and RG)
6. Previous numerical simulations.
7. Our numerical simulations
8. Conclusions

Surfaces

The free energy of a surface

$$F = \mu N - pV + \sigma A$$

can be written on a more general way:

$$F = \left(\frac{\mu}{v} - p\right) \int \int dx dy h(x, y) + \int \int dx dy \phi(h_x, h_y) .$$

μ is the chemical potential, $v = V/N$, $h(x, y)$ is the height of the surface at the point of coordinates (x, y) , p is the pressure and $\phi(h_x, h_y) = \sigma(h_x, h_y) \sqrt{1 + h_x^2 + h_y^2}$, σ being the surface tension.

Working at a constant pressure, we can study the influence of

- The surface tension.
- The chemical potential.

Diffusion in surfaces: The chemical potential

The chemical potential of the surface is modified following the law (for a smooth surface)

$$\mu = \mu_0 - a\nabla^2 h$$

where μ_0 is the equilibrium chemical potential of the solid (under the hypothesis of local equilibrium). So, a terrace has a higher chemical potential, and the chemical potential of a hole is lower (i.e. higher curvature has a large chemical potential). A flat surface has the chemical potential of the solid at equilibrium.

Hence, the chemical potential induces diffusion from higher chemical potential regions to low chemical potential ones. The current (only on the surface) is then

$$\mathbf{j} = -D_s \nabla \mu$$

and the continuity equation (the number of particles is constant)

$$\frac{\partial h}{\partial t} = -\nabla \mathbf{j}$$

and then

$$\frac{\partial h}{\partial t} = D_s \nabla^2 \mu = -\kappa (\nabla^2)^2 h$$

$$\kappa > 0.$$

The main role of the chemical potential is to minimize the mean curvature.

Evaporation in Surfaces: Surface Tension

Assuming that the chemical potential of the vapor is uniform μ_0 , there will be evaporation in places where $\mu > \mu_0$.

We can assume that the variation of the height with time is linear with the chemical potential difference:

$$\frac{\partial h}{\partial t} \propto -(\mu - \mu_0)$$

and so

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h$$

with $\nu > 0$.

The main role of the surface tension is to minimize the area of the surface.

The continuum model

Taking into account evaporation, surface diffusion and thermal fluctuations we can write the following Langevin equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h - \kappa (\nabla^2)^2 h + \eta(\mathbf{r}, t)$$

where $\eta(\mathbf{r}, t)$ is a Gaussian noise.

The characteristic time of the q mode is:

$$\frac{1}{\tau(q)} = \nu q^2 + \kappa q^4$$

Hence, for small momenta (critical region) the surface tension always dominates. The crossover length is

$$L_c = \sqrt{\frac{\kappa}{\nu}}$$

For $L < L_c$ the system behaves tensionless.

If $\nu = 0$ the model has not a well defined thermodynamic limit when the substrate dimension is 2 (in 2+1 dimensions). The height-height correlation function diverges even if we compute it at finite distances:

$$C(r) \equiv \langle (h(\mathbf{r}) - h(0))^2 \rangle \rightarrow \infty \text{ as } L \rightarrow \infty$$

Moreover we can define the slope-slope correlation function:

$$C_d(s) \equiv \langle (\nabla h(\mathbf{r} + \mathbf{s}) - \nabla h(\mathbf{r}))^2 \rangle$$

The discrete model

If we take into account the discrete character of the surface, we can write two related models:

$$\mathcal{H} = \nu \sum_{\mathbf{r}} [\nabla_d h(\mathbf{r})]^2 + \kappa [\nabla_d^2 h(\mathbf{r})]^2$$

∇_d is the discrete gradient and $h \in Z$.

Its continuum limit is well described by the modified sine-Gordon model:

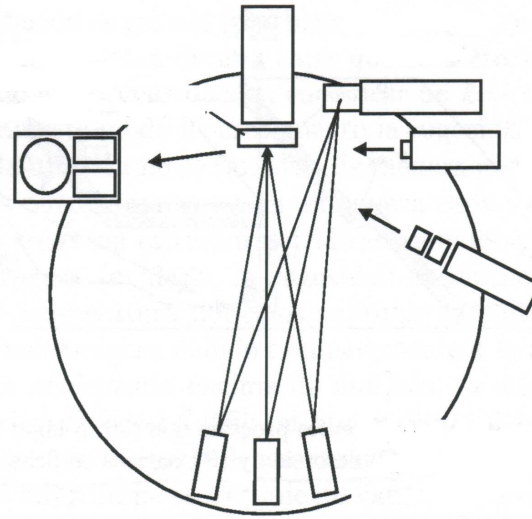
$$\mathcal{H} = \int d^d r (\nu [\nabla h(\mathbf{r})]^2 + \kappa [\nabla^2 h(\mathbf{r})]^2 + V (1 - \cos(2\pi h(\mathbf{r}))))$$

Now, $h \in R$.

When $\kappa = 0$ the model undergoes, in two dimensions, the roughening transition (in the KT universality class):

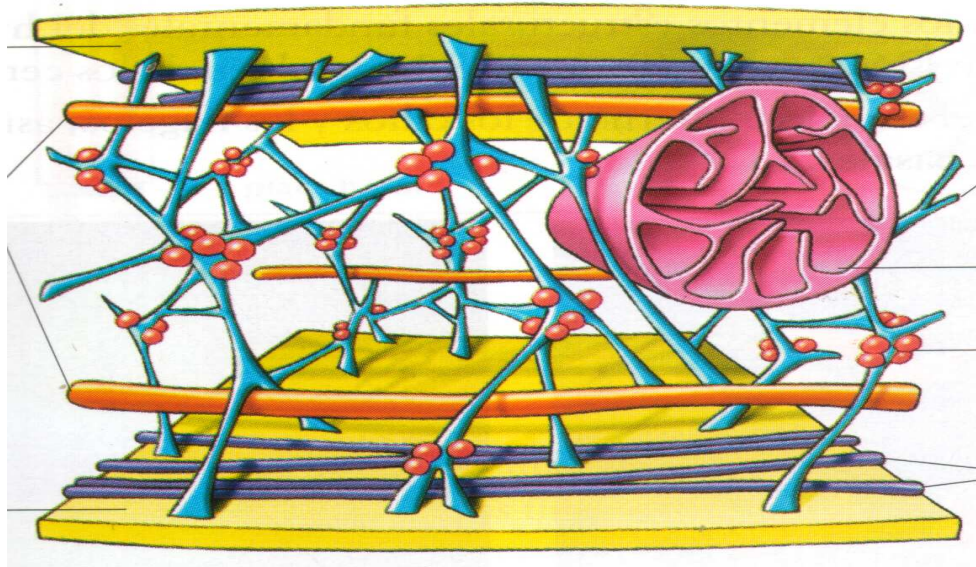
- $T < T_R$, $C(r) \simeq e^{-r/\xi}$. Flat surface. Massive phase.
- $T > T_R$, $C(r) \simeq \log r$. Rough surface. Massless phase.
- $\xi(T) \simeq \exp \left[-\frac{C}{\sqrt{T_R - T}} \right]$, as $T \rightarrow T_R^-$. Phase transition of infinite order.
- $T_R(L) = T_R + a/(\log L + b)^2$.

Example I : Molecular Beam Epitaxy



- Process of great importance in technology.
- In most MBE processes there are not evaporation, e.g. Nickel.
- But in GaAs, arsenic evaporates!!

Example II: Biological Membranes



A fluid membrane (e.g. the lipid membrane) is a good example of tensionless surface. The lipid fluid is above its melting temperature, and can move on the surface.

Model of Gov and Sofran. They model the coupling between the elastic cytoskeleton by

$$\kappa(\nabla^2)^2\chi(r) + V(r)\chi(r) = 0 .$$

$\chi(r) = \langle h(r) \rangle$, and V introduces into the model the pinning of the surface by the cytoskeleton.

Example III: Two dimensional melting

Nelson proposed the discrete bilaplacian as a model for the two dimensional melting.

- By using the Poisson summation formula the discrete bilaplacian can be written like a Coulomb gas.
- Using the most relevant terms in the modified Coulomb gas a sequence of two KT transitions (scenario HNYKT) were found:
 1. $T > T_{c1}$: $C(r) \propto r^2 \log r$, $C_d(r) \propto \log r$.
 2. $T_{c1} > T > T_{c2}$: $C(r) \propto \log r$, $C_d(r) \propto 1$.
 3. $T < T_{c2}$: $C(r) \propto 1$, $C_d(r) \propto 1$.

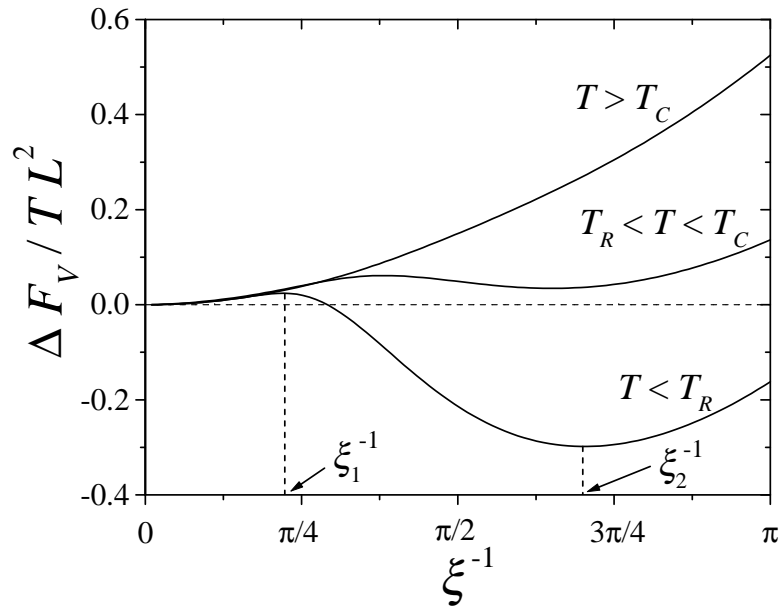
Variational Approach

The starting point is the Bogoliubov-Feynman inequality:

$$\mathcal{F} \leq \mathcal{F}_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0$$

$$\mathcal{H}_0 \equiv \frac{T}{2} \sum_{\mathbf{q}} S^{-1}(\mathbf{q}) h_{\mathbf{q}} h_{-\mathbf{q}}$$

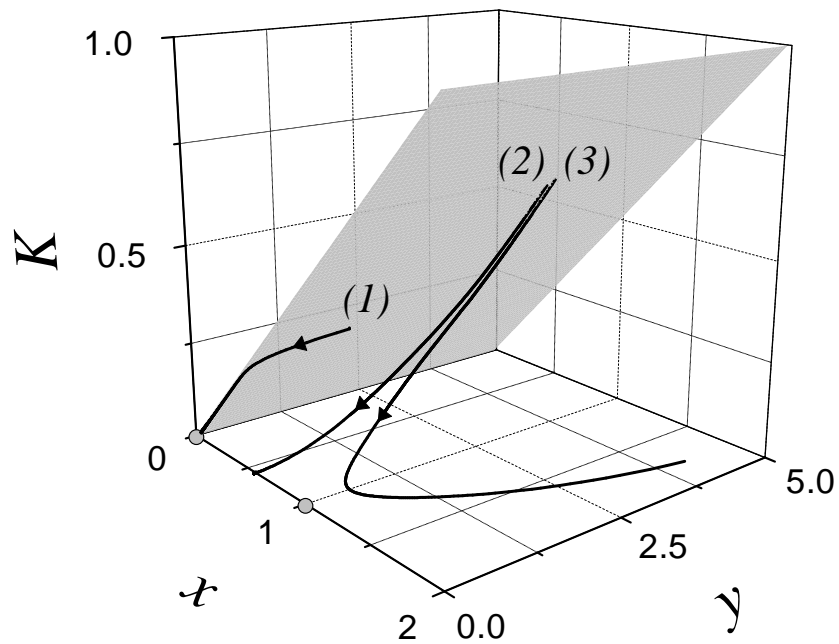
$d = 2$ $\Delta \mathcal{F} \equiv \mathcal{F}_\xi - \mathcal{F}_{\xi=\infty}$



First Order Phase Transition. $\left(\begin{array}{c} T \rightarrow T_R^- \\ \xi \longrightarrow \text{const.} \end{array} \right)$

Renormalization Group Approach

- Renormalization of the Langevin equation. Scheme of Nozières-Gallet.
- $L_c(l) = \sqrt{\kappa(l)/\nu(l)}$, $l = \log b$, b being the scale factor in RG.
- If $L < L_c(l)$: tensionless surface.
- If $L > L_c(l)$: surface with surface tension.



For large lattices, we will always have surface tension.

Numerical Simulations

Previous Numerical Simulations

- Numerical simulations by Bruce confirms the Nelson scenario with $T_{c1} = 2.2$ and $T_{c2} = 1.64$.
- Simulations by Janke and Kleinert in a modified model implies a first order phase transition in the bilaplacian model at $T_c = 2.454$.

Our numerical simulations

1. Standard Metropolis algorithm.
 2. Linux PC cluster.
 3. $L < 128$. Some runs $L = 256$.
 4. We compute local quantities, energy, τ , and global ones: correlations functions.
 5. We have done some dynamical studies.
- The system behaves in a bilaplacian way at $T = 1.8$ so the Bruce and Janke and Kleinert scenarios cannot be right.
 - The system undergoes a continuous phase transition near $T = 1.64$ (where the system develops a not diverging specific heat peak) between a high temperature phase well describe by the bilaplacian and a low temperature one which can be described by a massive quadratic propagator.
 - $\alpha \leq 0$ and $\nu \simeq 0.7$ violate hyperscaling ($\alpha = 2 - \nu d$), so
 - We [conjecture](#) that the phase transition is in the [KT universality class](#).

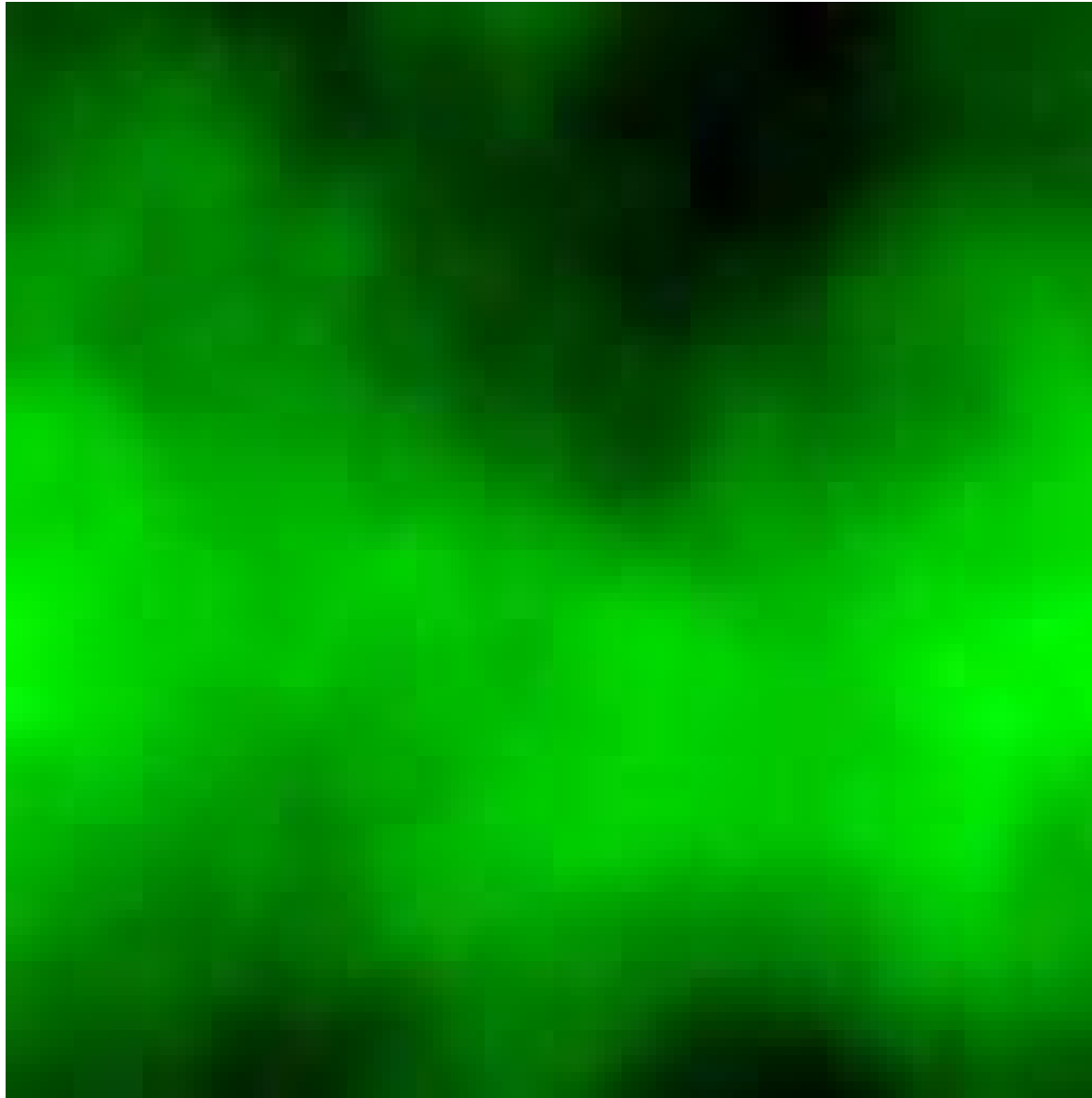


Figure 1: A configuration $T = 2.0$

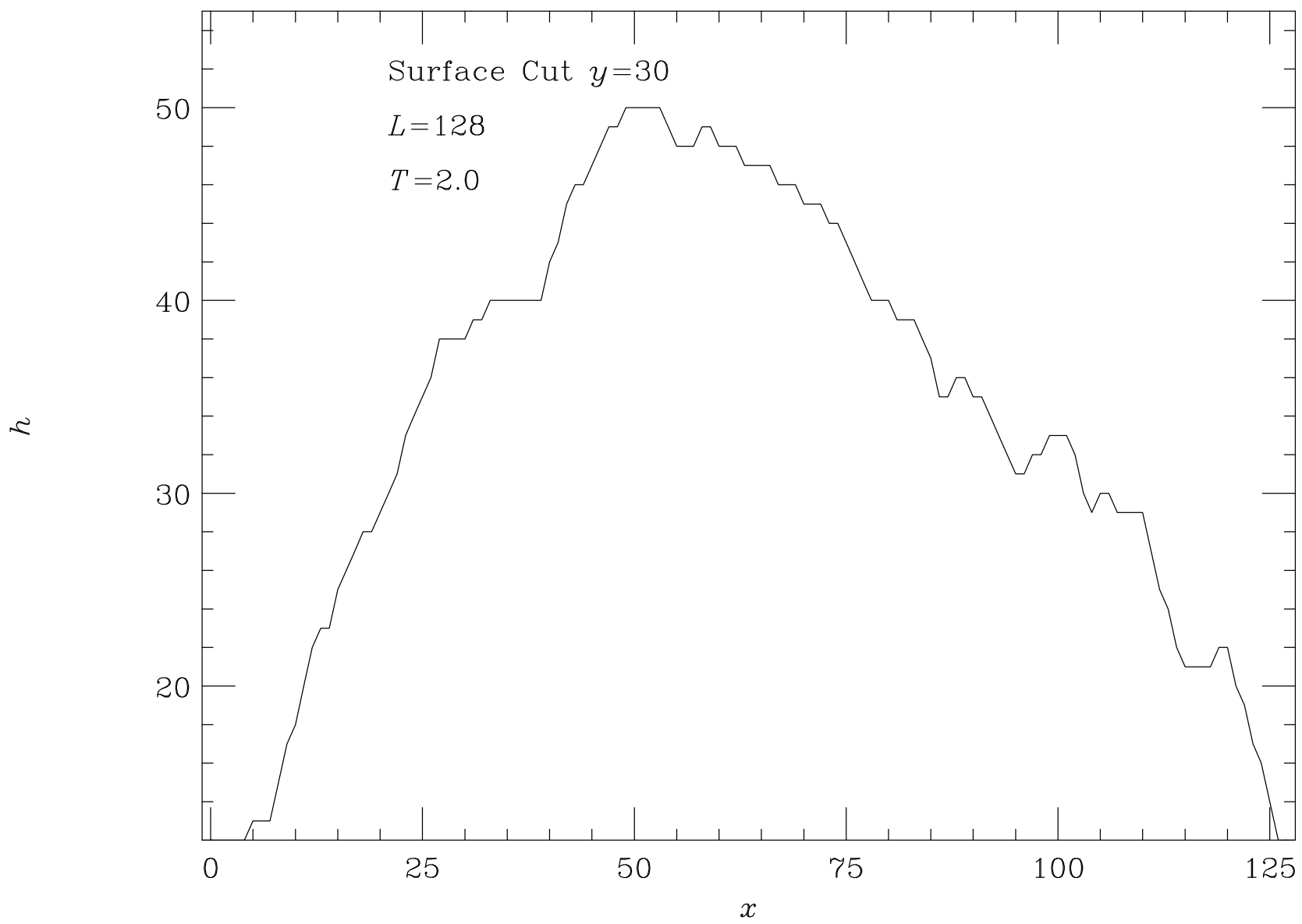


Figure 2: Cut of a configuration $T = 2.0$

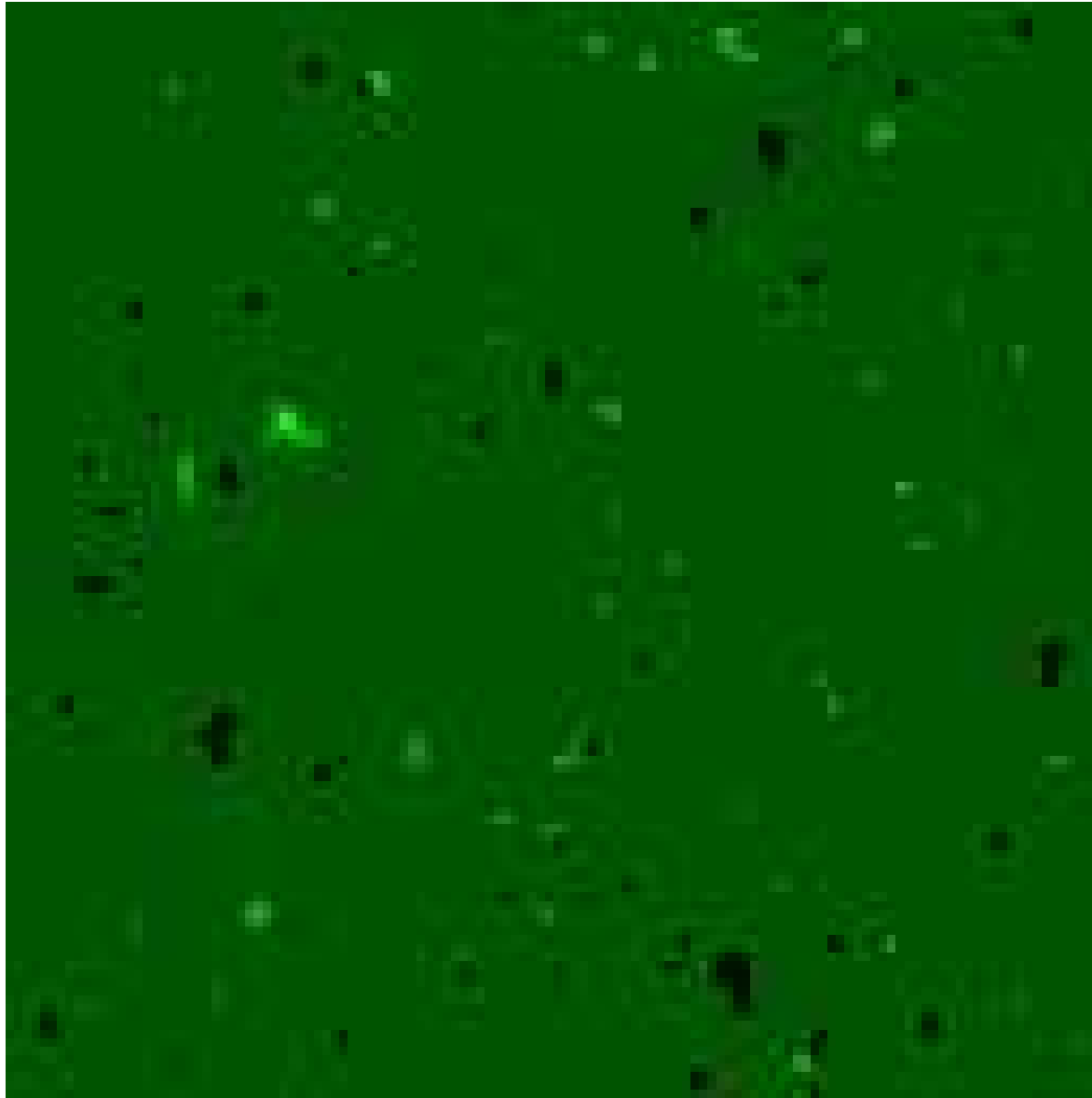


Figure 3: A configuration $T = 1.5$

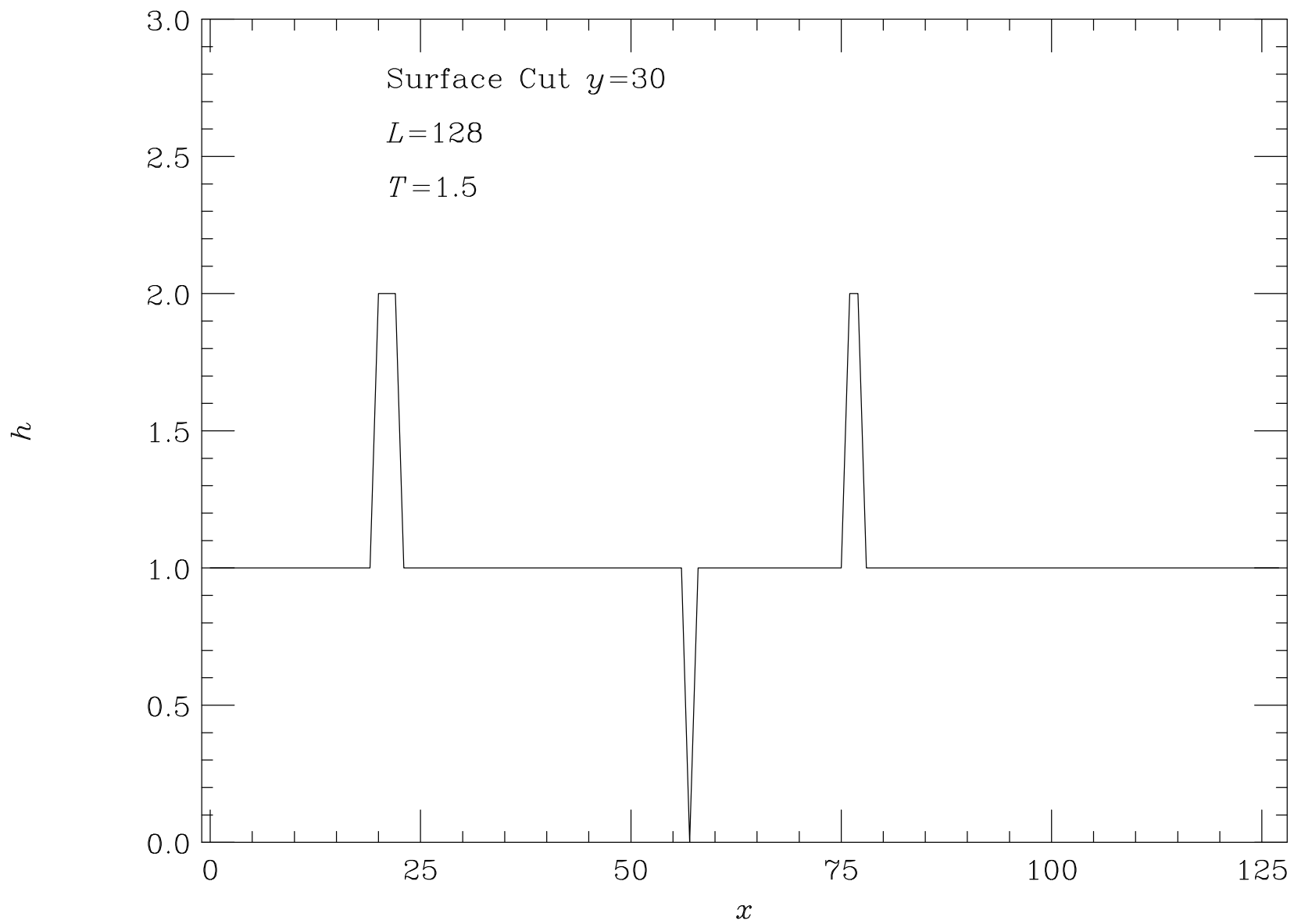


Figure 4: Cut of a configuration $T = 1.5$

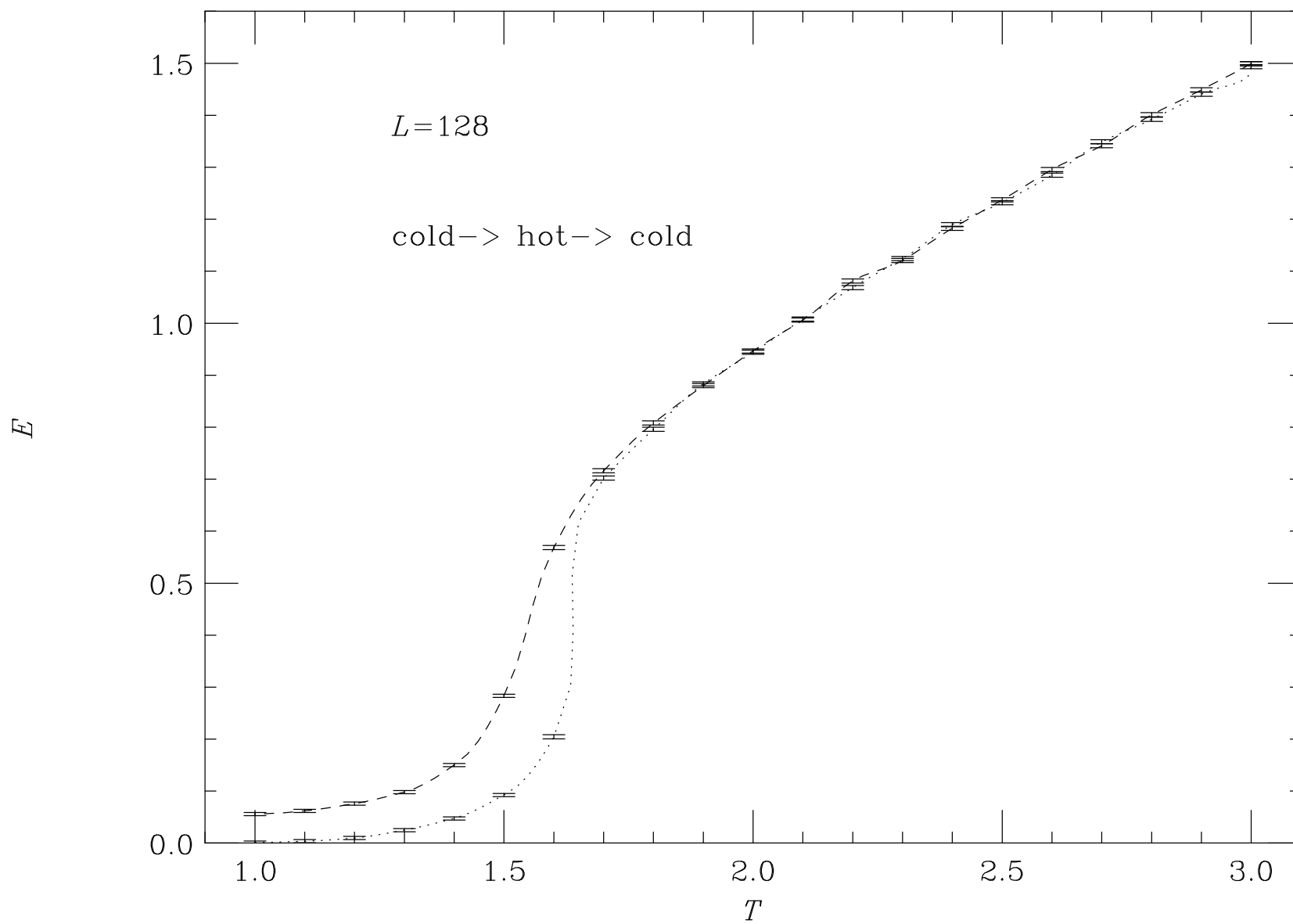


Figure 5: Energy. Annealing schedule. Cold-Hot-Cold

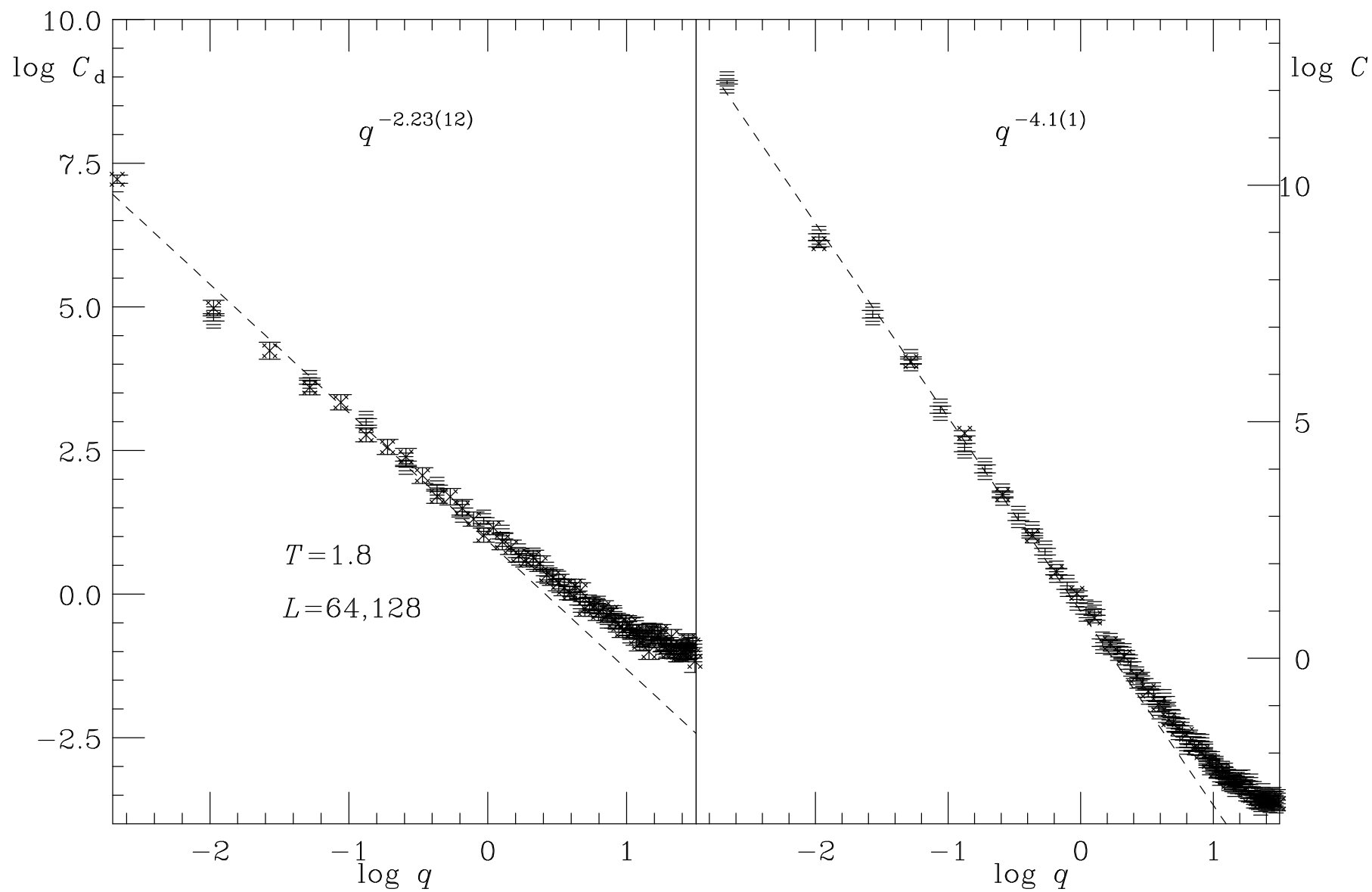


Figure 6: Propagators. $T = 1.8$

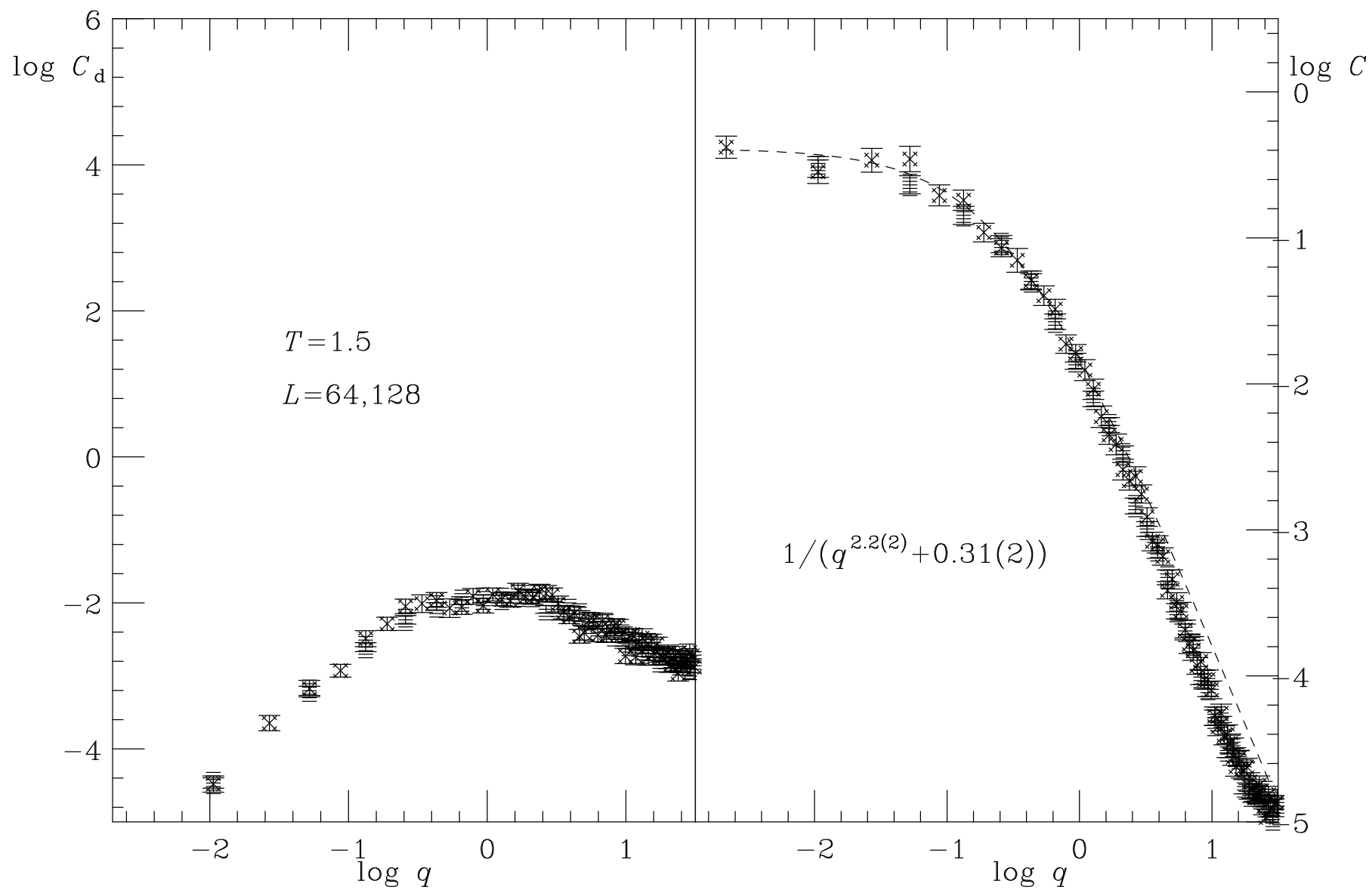


Figure 7: Propagators. $T = 1.5$

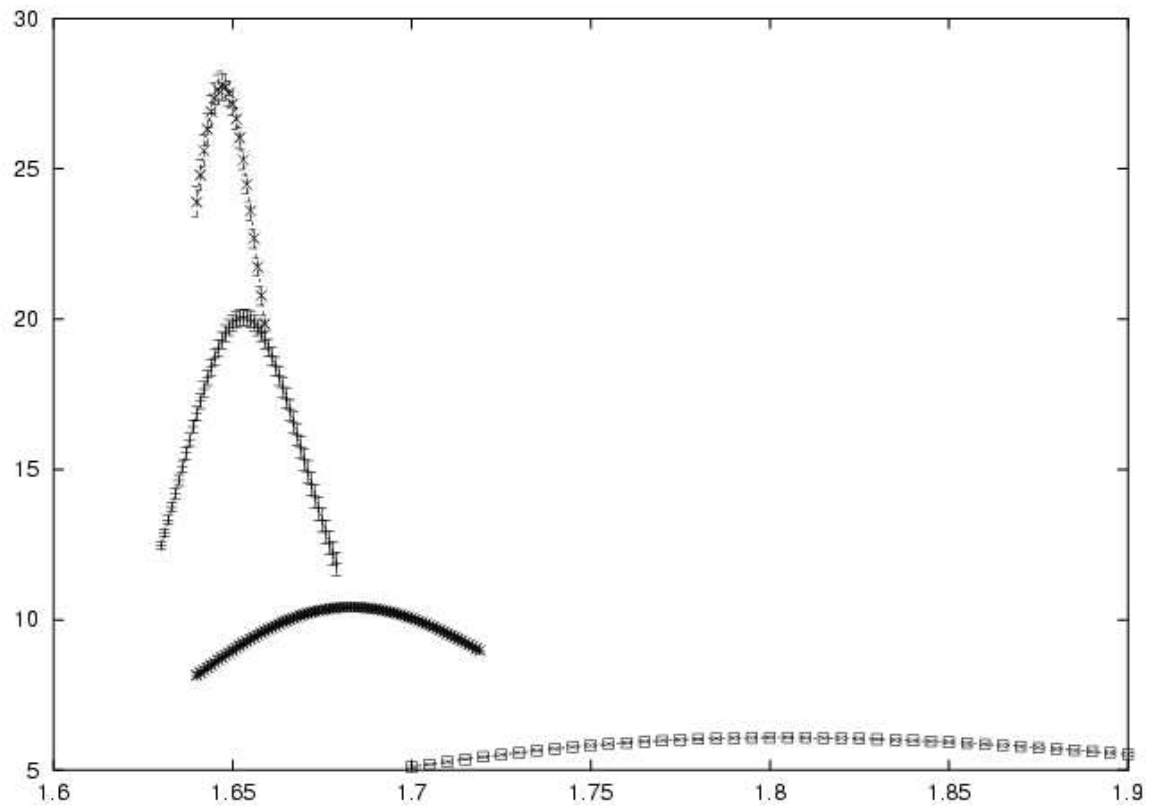


Figure 8: Specific Heat for the smaller lattices as a function of T .

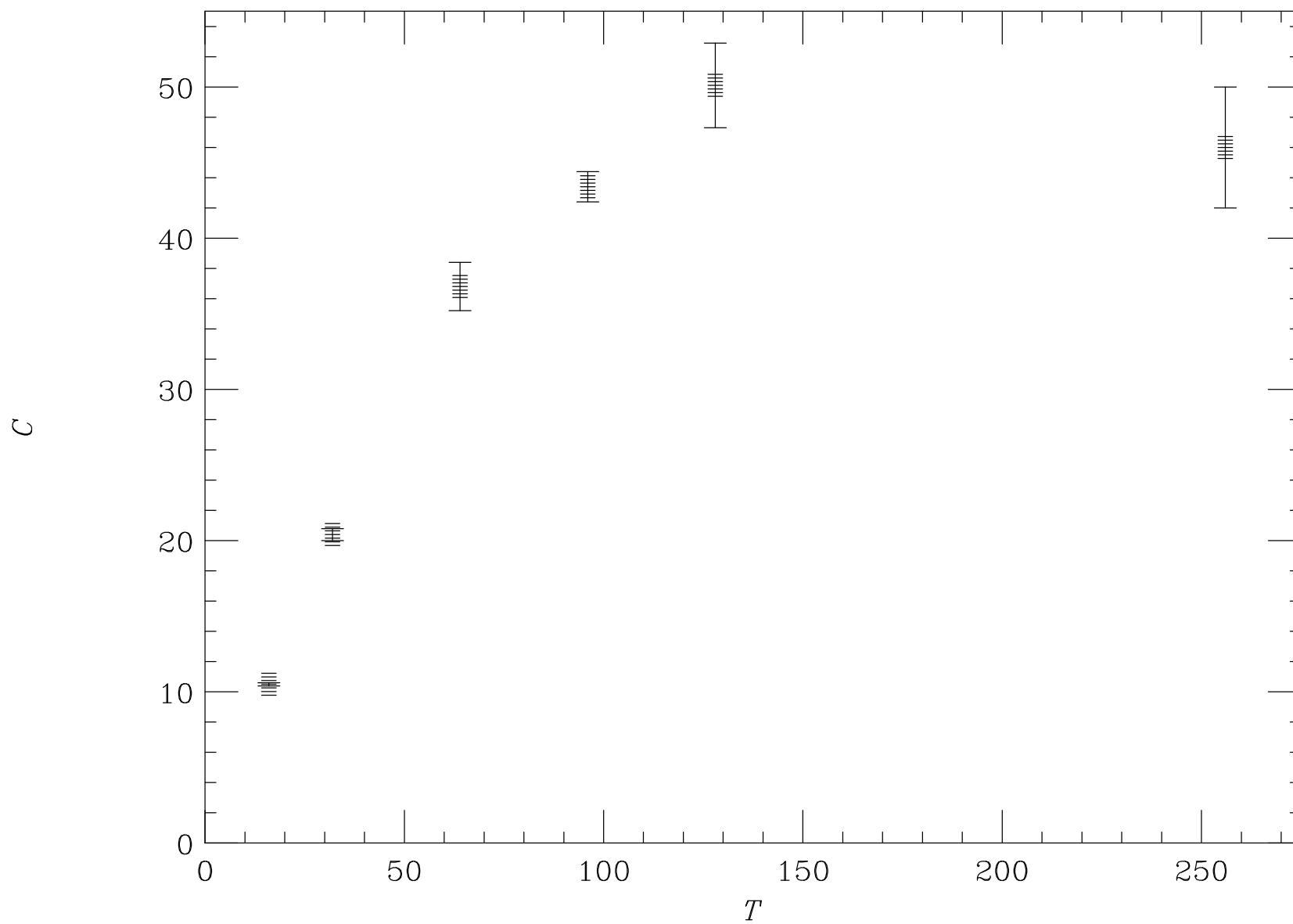


Figure 9: Peak Specific Heat as a function of L .

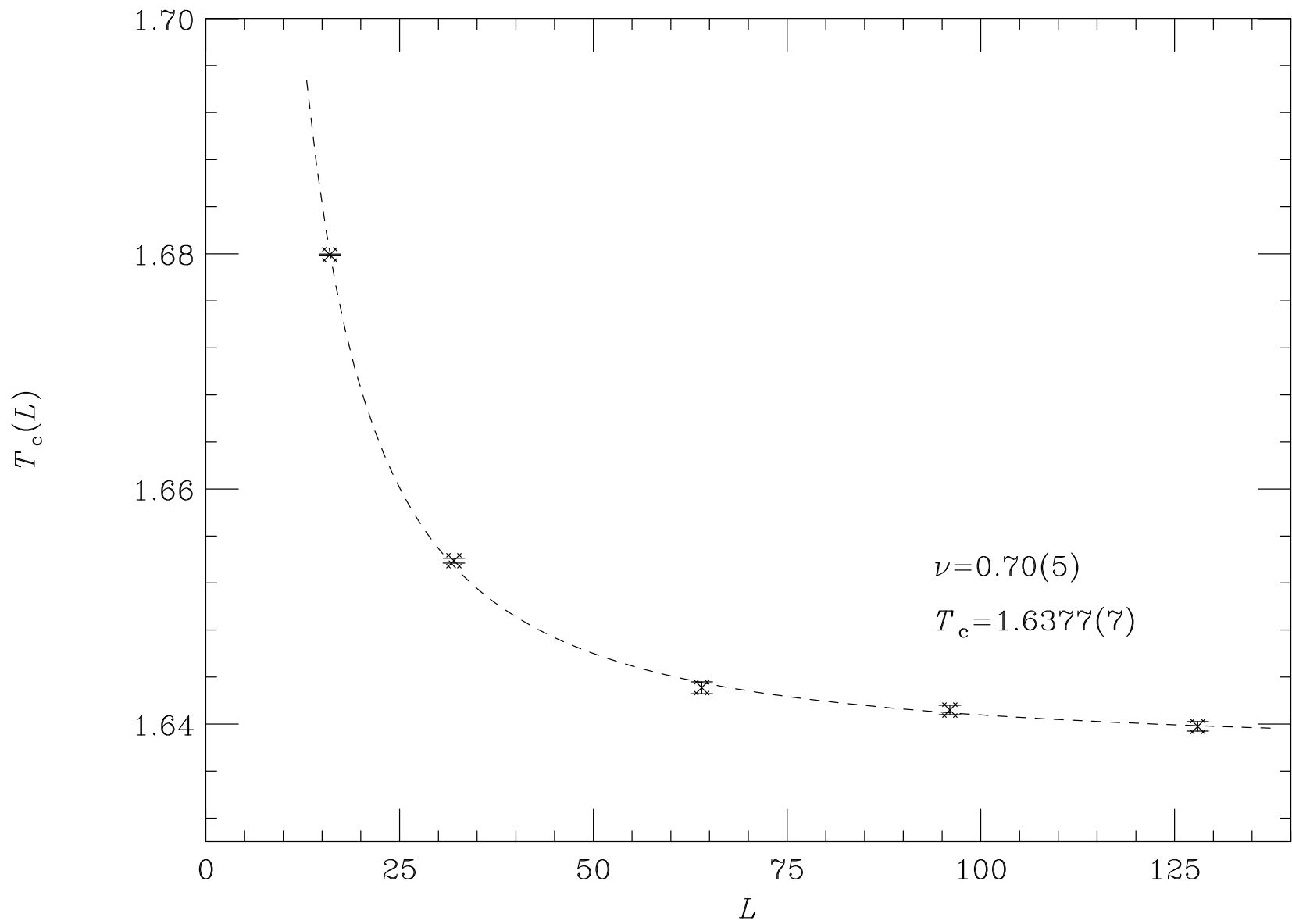


Figure 10: $T_c(L)$ as a function of L .

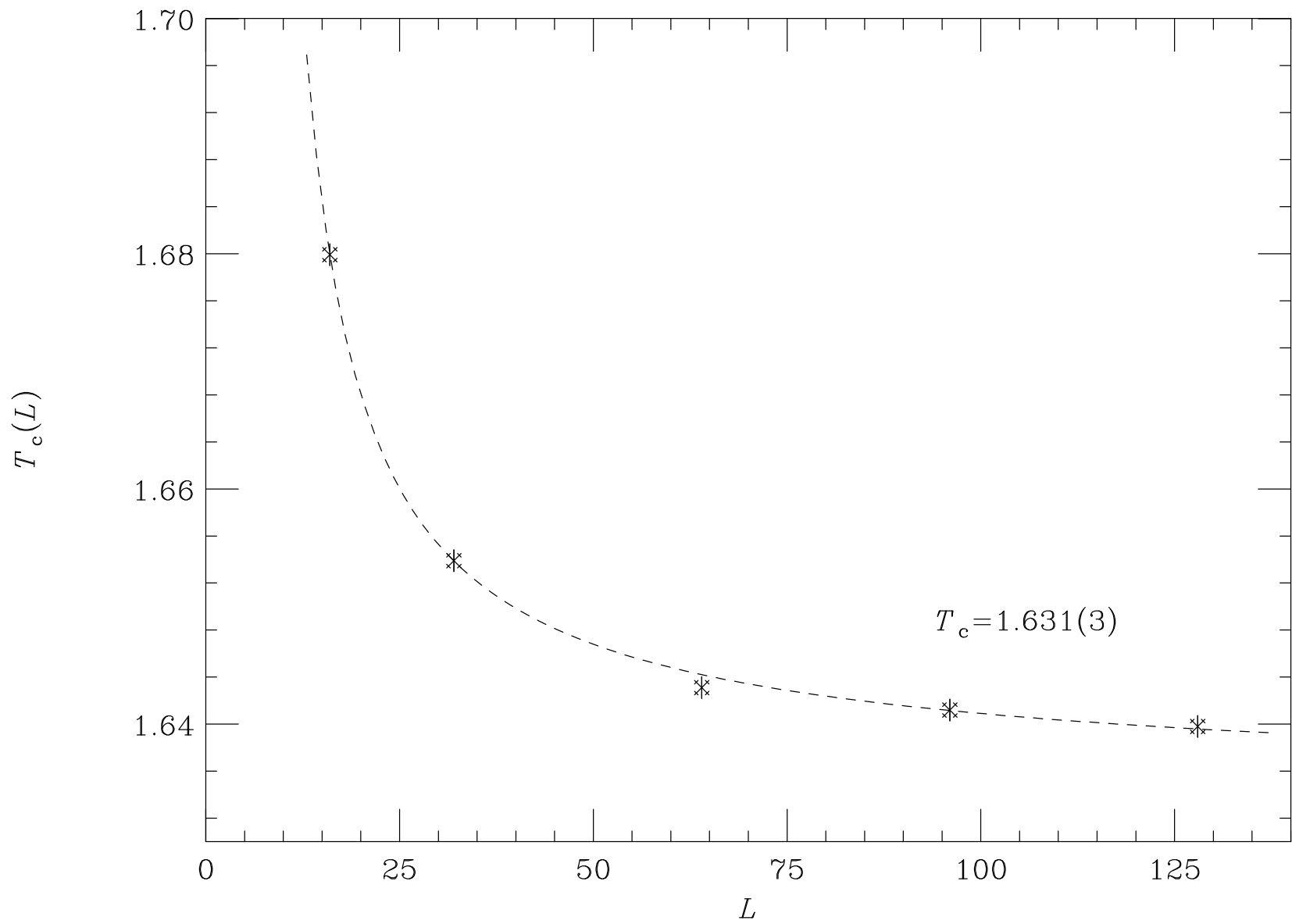


Figure 11: $T_c(L)$ as a function of L .KT scenario.