Long-Range Interactions and Dynamics in Complex Quantum Systems

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First-order and second-order phase transitions in a quantum Nagle-Kardar model

Alessandro Campa

ISS and INFN, Roma, Italy

In collaboration with Andrea Trombettoni

Trieste University and ICTP, Italy

Outline

- The model and its various integrable limits
- The approximations used in its study
- Thermodynamic phase diagram
- Conclusions and perspectives

The motivation is to study the influence of quantum fluctuations in systems where the presence of competing interactions causes a complex thermodynamic phase diagram and ensemble inequivalence.

We consider a 1D Ising spin system with both long-range (mean-field) and short-range (nearest-neighbour) interactions in a transverse field.

The Hamiltonian is

$$H = -\frac{J}{2N}\sum_{i,j}\sigma_i^z\sigma_j^z - \frac{K}{2}\sum_i \sigma_i^z\sigma_{i+1}^z - h\sum_i \sigma_i^x \,,$$

where the σ's are the Pauli matrices, and the sums on i and j are from 1 to N.

Let us first consider the various limits where one of the coefficients vanishes.

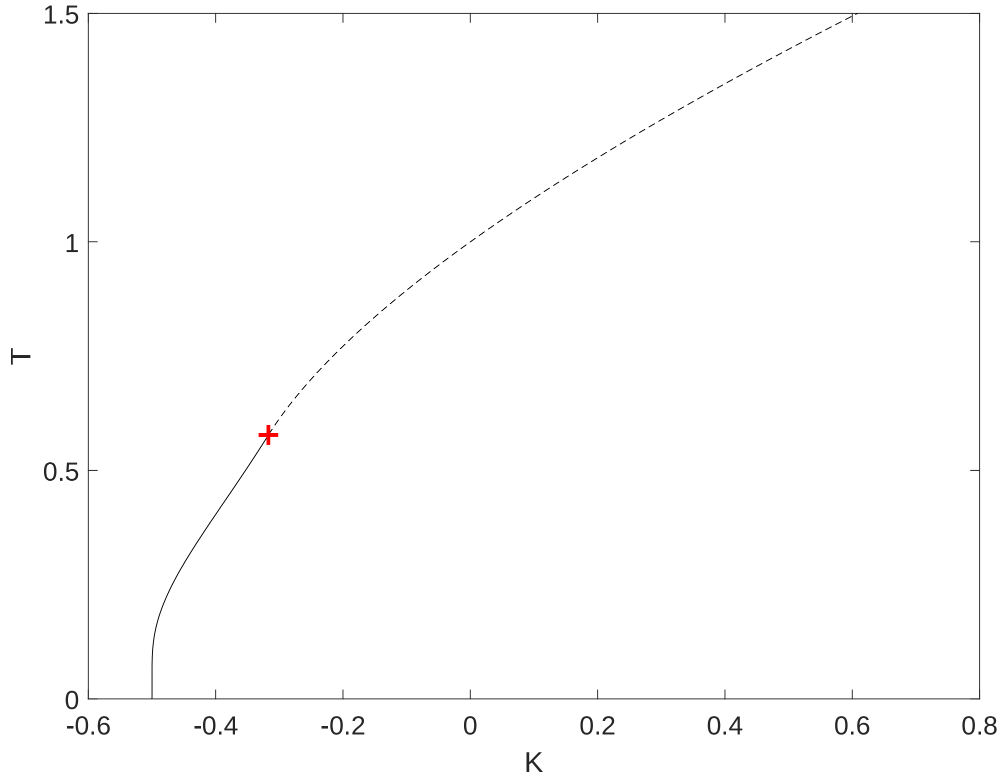
When the transverse field h vanishes we have the classical Nagle-Kardar model

$$H = -\frac{J}{2N}\sum_{i,j}\sigma_i^z\sigma_j^z - \frac{K}{2}\sum_i \sigma_i^z\sigma_{i+1}^z,$$

whose partition function can be easily obtained. In the thermodynamic limit the free energy per spin as a function of the inverse temperature β is

$$f = \min_x\left\{\frac{x^2}{2} - \frac{1}{\beta}\ln\left[\mathrm{e}^{\frac{\beta K}{2}}\cosh(\beta x) + \sqrt{\mathrm{e}^{\beta K}\sinh(\beta x) + \mathrm{e}^{-\beta K}}\right]\right\}$$

Studying this function the thermodynamic phase diagram in the (K, T) plane can be obtained. It presents a line of first-order phase transitions and a line of second-order phase transitions; they are joined at a tricritical point. The transition is between a magnetized (ferromagnetic) state and an unmagnetized (paramagnetic) state.



1.5
1
0.5
0
T
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
K

When the mean-field coupling J vanishes we have the transverse field Ising model

$$H = -\frac{K}{2}\sum_i \sigma_i^z \sigma_{i+1}^z - h\sum_i \sigma_i^x \, .$$

It can be solved exactly with the Jordan-Wigner transformation. It presents a quantum second-order transition at $T = 0$, located at $K = 2h$. For positive T the system is paramagnetic, and there is no phase transition.

The last thing could be guessed on physical basis, since already the classical case ($h = 0$) is paramagnetic for positive temperatures, and we can expect this to be true a fortiori when the quantum fluctuations are added.

When the nearest-neighbour coupling K vanishes we get the Lipkin-Meshkov-Glick (LMG) model

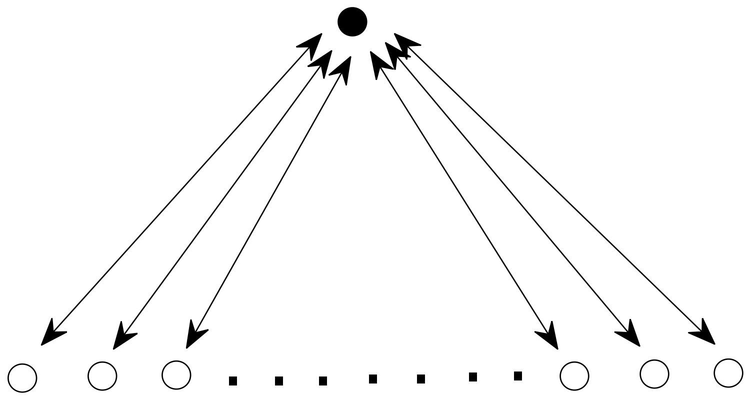
$$H = -\frac{J}{2N}\sum_{i,j}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^x\,.$$

The exact spectrum can be obtained with the Bethe ansatz. One exploits the fact that, defining $S^\alpha = \sum_i \sigma_i^\alpha$, the Hamiltonian takes the form

$$H = -\frac{J}{2N}(S^z)^2 - hS^x\,.$$

However, we are interested here in the thermodynamic limit $N \to \infty$. In this limit, it can be best seen as the $K = 0$ particular case of the solution of the full problem.

Before considering our Hamiltonian, we consider another model, in order to see the physical and mathematical relation with ours. In this other model, there is no long-range interaction, but each spin is coupled to an external degree of freedom.



The short-range part of the Hamiltonian is left unchanged. The external degree of freedom could be, e.g., a magnetic field which is not fixed, but like the spins is a dynamical variable.

The Hamiltonian of this model would be

$$\widetilde{H} = \frac{1}{2}ax^2 - ax\sum_i \sigma_i^z - \frac{K}{2}\sum_i \sigma_i^z\sigma_{i+1}^z - h\sum_i \sigma_i^x \,,$$

with the first term representing the energy in the magnetic field and the second term the interaction of this field with the spins.

The partition function of this systems is

$$Z = \int \mathrm{d}x \, \mathrm{Tr}_{\{\sigma\}} \exp\left[-\beta\widetilde{H}\right]$$

Let's write this Hamiltonian in the more general form

$$\widetilde{H} = \frac{1}{2}ax^2 - ax\sum_i \sigma_i^z + H_s \,,$$

where H_s is a generic Hamiltonian with only short-range interactions.

If one neglects the commutator $[\sum_i \sigma_i^z, H_s]$ the partition function becomes, apart from a multiplicative coefficient,

$$Z = \mathrm{Tr}_{\{\sigma\}} \exp\left[-\beta H\right] \ ,$$

where the Hamiltonian H is

$$H = -\frac{a}{2} \sum_{i,j} \sigma_i^z \sigma_j^z + H_s \, .$$

Therefore we would have the same partition function of a system described by H_s plus a mean-field interaction.

This fact is exploited in classical systems, where the variable x is not interpreted as the dynamical variable of a related system, but simply as a dummy variable in what is called the Hubbard-Stratonovich transformation.

Let'see what we can do in quantum systems.

For a finite system, neglecting the commutator is for sure an approximation that one introduces in the computation of the partition function, that therefore has to be interpreted as the partition function of the Hamiltonian $\widetilde{H}$, that describes the related model with the additional dynamical variable x and without the long-range interaction. But we are interested in the thermodynamic limit.

First of all in our case the coefficient a in the Hamiltonian $\widetilde{H}$ must be equal to J/N. Without loss of generality from now on we take $J = 1$. So we have

$$\widetilde{H} = \frac{1}{2N}x^2 - \frac{1}{N}x\sum_i \sigma_i^z + H_s\,.$$

Since we have to integrate over x we can make $x \to Nx$ (this introduces a factor proportional to $(\ln N/N)$ in the free energy per spin, that vanishes in the TL)

$$\widetilde{H} = \frac{N}{2}x^2 - x\sum_i \sigma_i^z + H_s\,.$$

Then we have

$$Z = \int \mathrm{d}x \, \mathrm{Tr}_{\{\sigma\}} \exp\left[-\frac{\beta N}{2N} x^2 + \beta x \sum_i \sigma_i^z - \beta H_s \right]$$

Up to now we have not yet done anything essential to solve the problem of the commutator $[\sum_i \sigma_i^z, H_s]$. The thermodynamic limit $N \to \infty$ helps us since the above integral in x is dominated (saddle point) by a value $x \sim (1/N)\langle \sum_i \sigma_i^z \rangle$.

The approximation then is done to substitute this expectation value with the operator itself. In doing so, the effective Hamiltonian becomes the long-range Hamiltonian.

In conclusion, while in the classical case the Hubbard-Stratonovich transformation is exact for any N, in the quantum case it becomes exact only in the thermodynamic limit. It is to be noted that also in the classical case at the end one uses a saddle point approximation.

Therefore for our model

$$H = -\frac{1}{2N} \sum_{i,j} \sigma_i^z \sigma_j^z - \frac{K}{2} \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x \,,$$

we can write

$$Z = \int \mathrm{d}x \, \mathrm{Tr}_{\{\sigma\}} \exp\left[-\frac{\beta N}{2} x^2 + \beta x \sum_i \sigma_i^z + \frac{\beta K}{2} \sum_i \sigma_i^z \sigma_{i+1}^z + \beta h \sum_i \sigma_i^x \right] \,.$$

At this point the case $K = 0$ can be computed easily, since the traces over the different spins decouple. One obtains

$$Z = \int \mathrm{d}x \, \exp\left\{ -N \left[\frac{\beta}{2} x^2 - \ln(2\cosh[\beta\sqrt{x^2 + h^2}]) \right] \right\} \,.$$

This is computed with the saddle point, and the corresponding x, realizing the maximum of the exponent, gives the value of the order parameter $m = \frac{1}{N} \sum_i \langle \sigma_i^z \rangle$ at equilibrium.

One finds that for $h > 1$ the solution is $m = 0$, i.e., the system is paramagnetic, while for $h < 1$ there is a critical value β_c. For $\beta < \beta_c$ the system is again paramagnetic ($m = 0$), while for $\beta > \beta_c$ the order parameter is given by the solution of the equation

$$\sqrt{m^2 + h^2} = \tanh[\beta\sqrt{m^2 + h^2}]$$

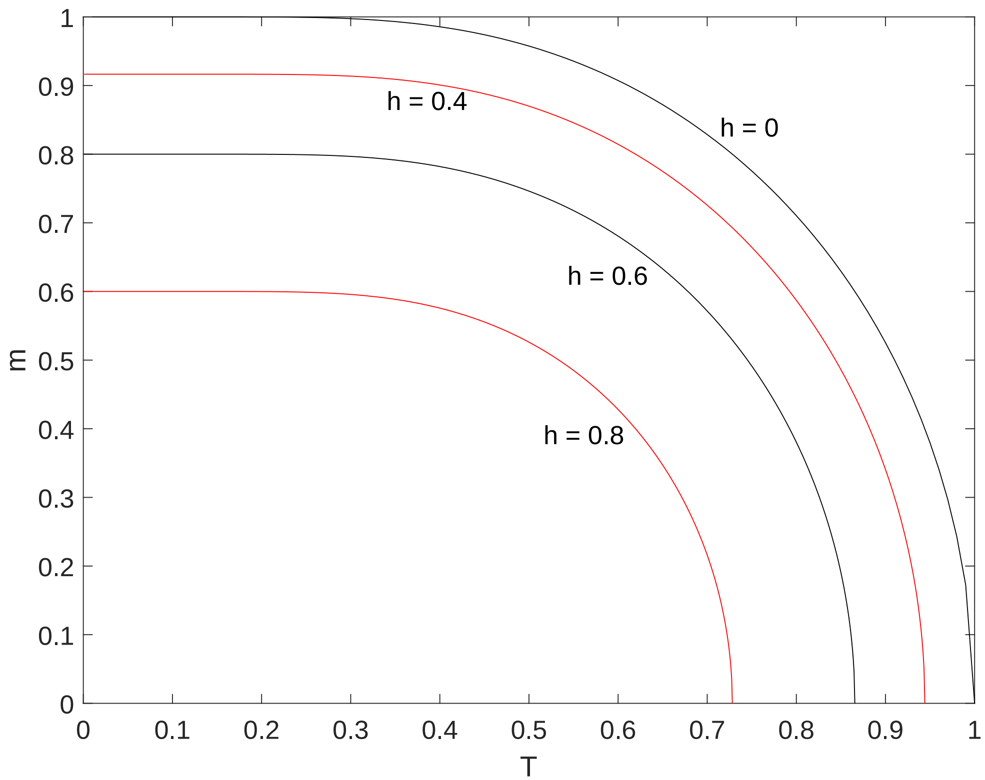
The value of β_c, at which there is a second-order phase transition, is given by

$$\tanh(\beta_c h) = h\,,$$

i.e.

$$\beta_c = \frac{1}{2h}\ln\frac{1+h}{1-h}\,.$$

$T_c = 1/\beta_c$ decreases from $T_c = 1$ for $h = 0$ to $T_c = 0$ for $h = 1$. For a given $h < 1$ the order parameter decrease from $\sqrt{1-h^2}$ at $T = 0$ to 0 at $T = T_c$.



h = 0
h = 0.4
h = 0.6
h = 0.8
m
T
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

The general case ($K \neq 0$) is less simple. As a matter of fact, we do not have an analytical formula for the computation of the trace.

We use the following series of approximations. We compute the partition function for a system in which one every p couplings between nearest-neighbour is removed.

The system is still fully connected by the mean-field interaction, but in the effective Hamiltonian the system decouples in block of p spins.

On physical grounds we expect that for increasing p the behaviour of the system approaches that of the original one ($p = \infty$).

The block structure of the effective Hamiltonian allows to compute the trace, at least for values of p for which the matrix dimension is manageable with respect to storage and computing time.

Therefore our partition function becomes

$$Z = \int \mathrm{d}x \, \exp\left[-\frac{\beta N}{2}x^2\right] \left\{ \mathrm{Tr}_{\{\sigma_1,\dots,\sigma_p\}} \exp\left[\beta x \sum_{i=1}^{p} \sigma_i^z + \frac{\beta K}{2} \sum_{i=1}^{p-1} \sigma_i^z \sigma_{i+1}^z + \beta h \sum_{i=1}^{p} \sigma_i^x \right] \right\}^{\frac{N}{p}} .$$

Denoting

$$\mathrm{Tr}_{\{\sigma_1,\dots,\sigma_p\}} \exp\left[\beta x \sum_{i=1}^{p} \sigma_i^z + \frac{\beta K}{2} \sum_{i=1}^{p-1} \sigma_i^z \sigma_{i+1}^z + \beta h \sum_{i=1}^{p} \sigma_i^x \right] \equiv \exp\left[-\beta f_p(\beta x, \beta K, \beta h)\right] ,$$

then

$$Z = \int \mathrm{d}x \, \exp\left\{-N\left[\frac{\beta}{2}x^2 + \frac{1}{p}\beta f_p(\beta x, \beta K, \beta h)\right]\right\} .$$

We consider only even p, so that the disordered ground state of a block (for K negative and sufficiently large in modulus) has $m = 0$.

The above expression is computed with the saddle point. We have performed computations for $p = 6$, 8, 10 and 12.

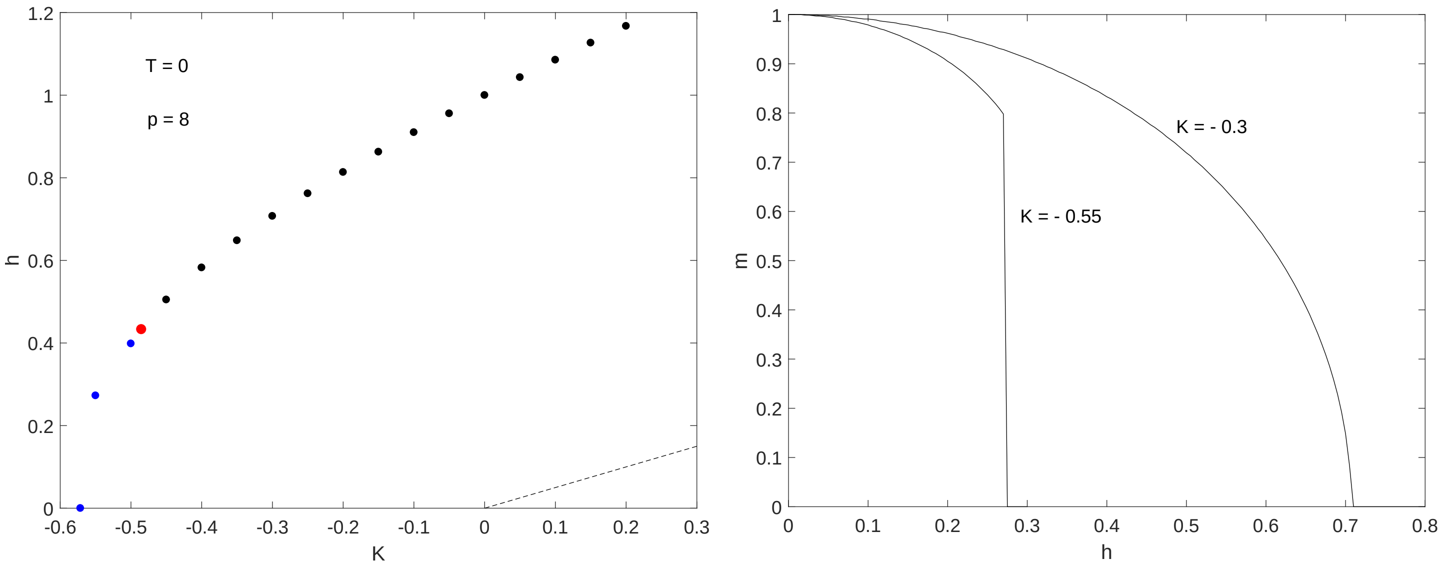
The saddle point evaluation gives

$$\beta f(\beta K, \beta h; p) = \min_x \left[\frac{\beta}{2} x^2 + \frac{1}{p} \beta f_p(\beta x, \beta K, \beta h) \right] .$$

The study of this function gives information on the presence of phase transitions.

The thermodynamic phase diagram is threedimensional (K, h, T). We present the results in 2D cuts defined by planes (K, T) at fixed values of h. This for the various values of p.

But first we show the phase diagram at $T = 0$ in the plane (K, h). It presents a line of first-order transitions and a line of second-order transitions joined at a tricritical point.



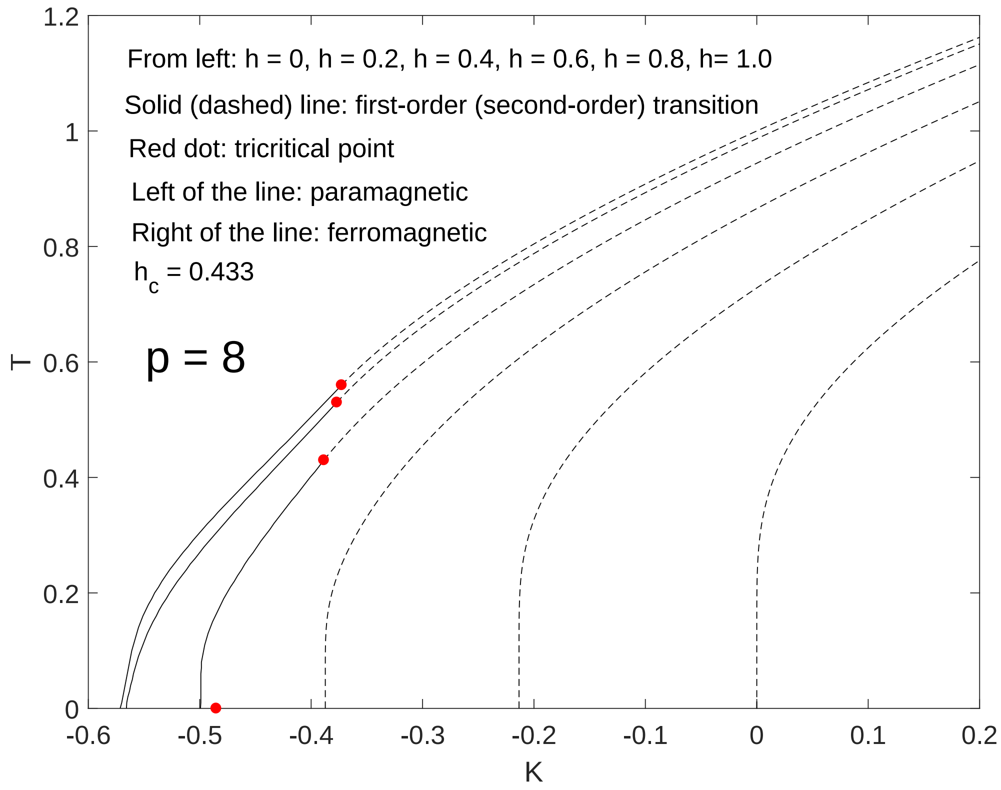
T = 0
p = 8
h
K
K = - 0.3
K = - 0.55
m
h

Intermission: first-order phase transitions and ensemble inequivalence.

The presence of first-order phase transitions in a long-range system implies inequivalence of the canonical ensemble with the microcanonical ensemble. In fact, the function $\beta f(\beta)$ is the Legendre-Fenchel transform of the microcanonical entropy, i.e.

$$\beta f(\beta) = \min_{\varepsilon} \left[\beta\varepsilon - s(\varepsilon)\right] \, ,$$

and as such it is a concave function. A discontinuity in $\beta f(\beta)$, i.e., a first-order phase transition, implies the presence of a convex part in the microcanonical entropy. In short-range systems this convex part is substituted by a linear section, related physically to phase separation, and this restores equivalence. This, however, does not occur in long-range systems, where there is no phase separation, and then we have ensemble inequivalence.



From left: h = 0, h = 0.2, h = 0.4, h = 0.6, h = 0.8, h= 1.0
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
h_c = 0.433
p = 8
T
K
1.2
1
0.8
0.6
0.4
0.2
0
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2

For $h = 0$ the point at $T = 0$ and the second-order line can be computed analytically. The point at $T = 0$ for generic p is at

$$K = -\frac{p}{2(p-1)}\,.$$

The second-order transition line is given implicitly by:

$$p\left(\beta \mathrm{e}^{\beta K} - 1\right) + \frac{\beta\left(1 - \mathrm{e}^{2\beta K}\right)}{2} + \frac{\beta\left(1 - e^{\beta K}\right)^2}{2} \tanh^{p-1}\left(\frac{\beta K}{2}\right) = 0\,.$$

For $p \to \infty$ it becomes

$$\beta \mathrm{e}^{\beta K} - 1 = 0 \qquad \text{i.e.} \qquad K = T \ln T$$

while for $K \to \infty$ we get

$$\beta \to \frac{1}{p}$$

The last result can be guessed on physical grounds, and as well we can argue that the same limit holds for any finite h.

Consider first the case $h = 0$.

$$H = -\frac{1}{2N} \sum_i (\sigma_i^z)^2 - \frac{K}{2} \sum_i{}' \sigma_i^z \sigma_{i+1}^z \,,$$

where the prime on the second sum means that one every p nearest-neighbour interaction is absent. When K is very large positive and the temperature is finite, we can assume that each block of p spins is aligned, and then we can write

$$H = -\frac{p}{2M} \sum_i^M (\sigma_i^z)^2 \,,$$

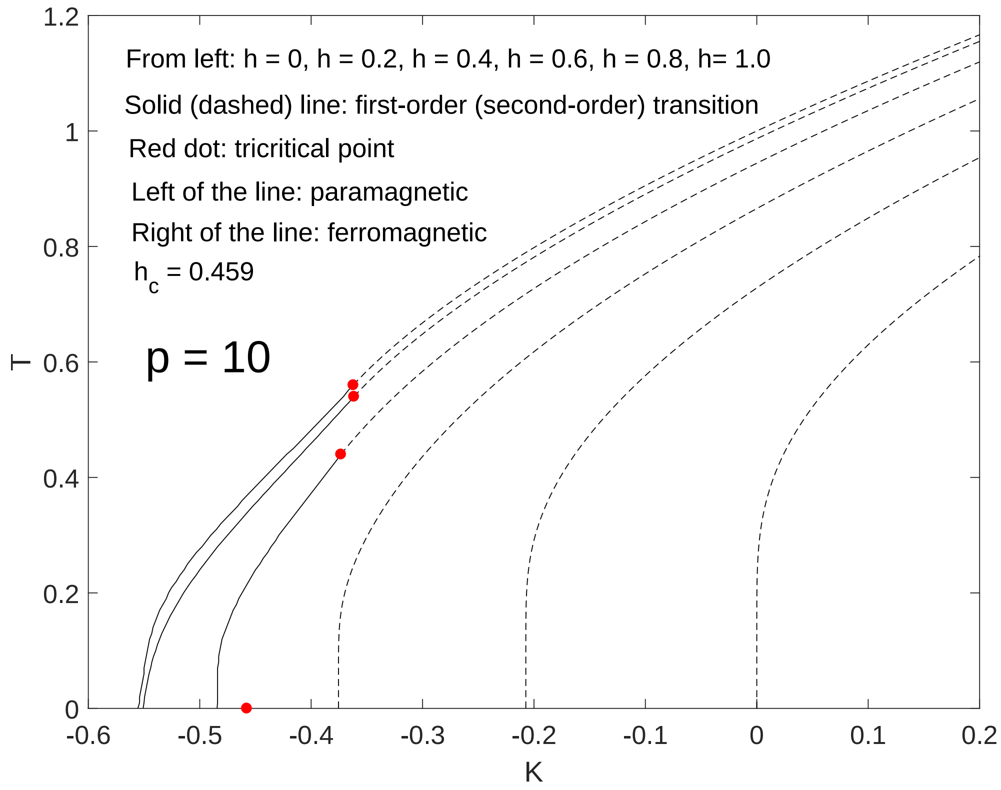
where $M = \frac{N}{p}$. This is the model with $K = 0$. We know that it has a second order transition at $T = 1$ when $J = 1$; therefore it has a second order transition at $T = p$ when $J = p$.

Consider now the case with $h > 0$ and finite, again with K very large positive

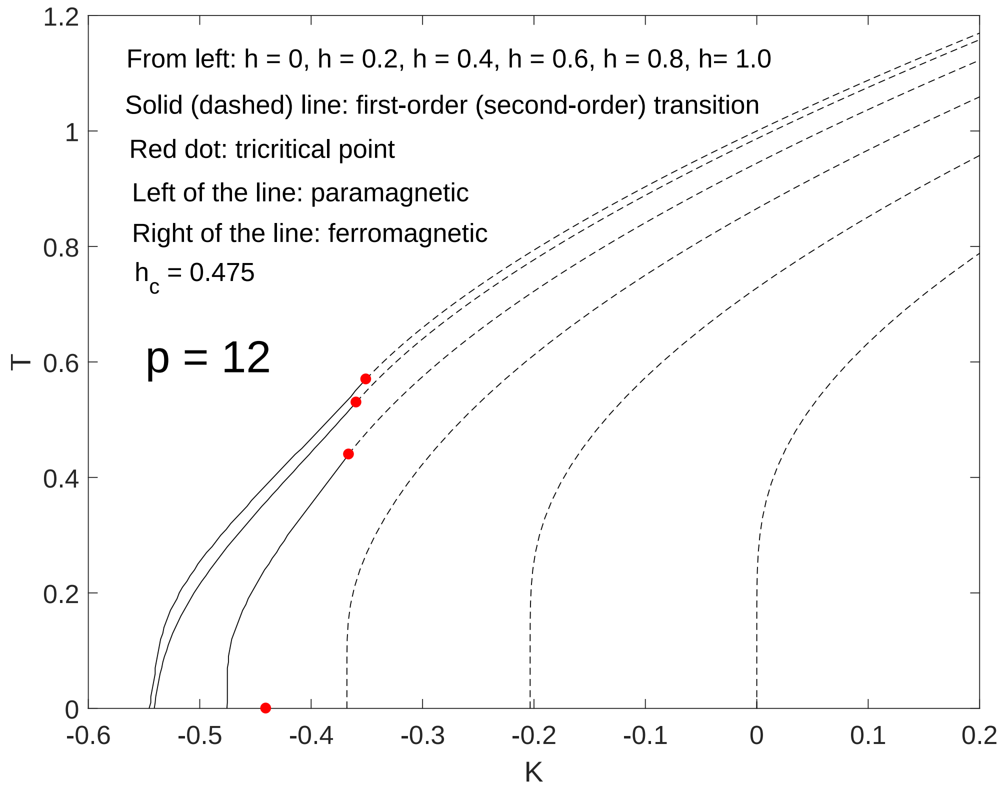
$$H = -\frac{1}{2N}\sum_i (\sigma_i^z)^2 - \frac{K}{2}\sum_i{}' \sigma_i^z \sigma_{i+1}^z - h\sum_i \sigma_i^x \,,$$

The last operator does not couples states where all p spins of a block are aligned in one direction with the states where they are aligned in the other direction. Therefore it does not change the leading eigenvalues of the spectrum. This implies that also in this case there is a second-order transition at $T = p$.

In conclusion, for large K the behaviour of the second-order line is very much dependent on p. We see shortly that this is in contrast to what happens for negative K, where the interesting things happen.



From left: h = 0, h = 0.2, h = 0.4, h = 0.6, h = 0.8, h= 1.0
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
h_c = 0.459
p = 10
T
K
1.2
1
0.8
0.6
0.4
0.2
0
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2

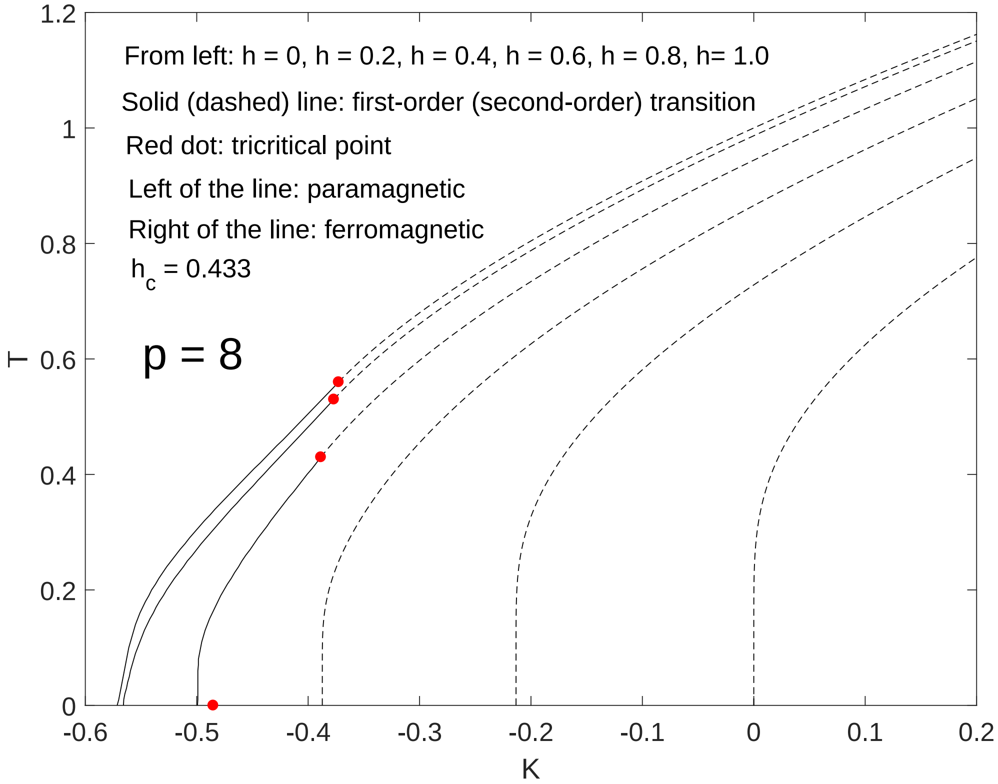

From left: h = 0, h = 0.2, h = 0.4, h = 0.6, h = 0.8, h= 1.0
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
h_c = 0.475
p = 12
T
K
1.2
1
0.8
0.6
0.4
0.2
0
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2

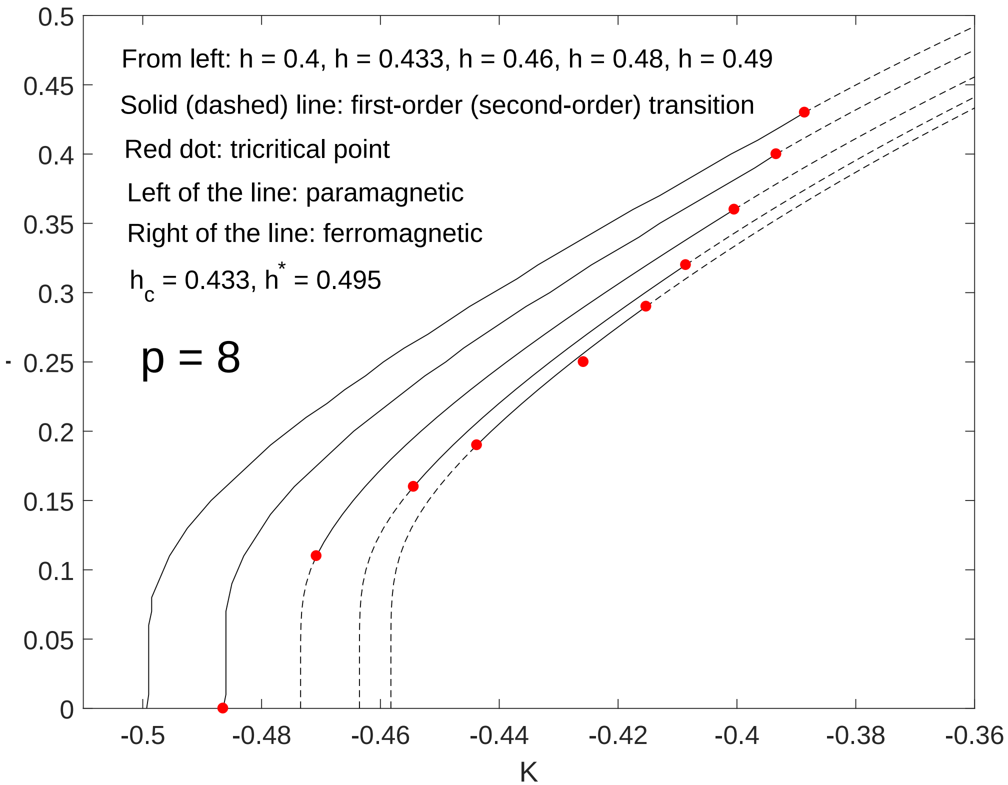
Therefore, for h less than a critical value h_c, the phase transition remains first-order for a range of temperatures, the range decreasing with h and vanishing for $h \to h_c$.

The task now is to try to infer, from our results, what could happen for $p \to \infty$, i.e., for the original model.

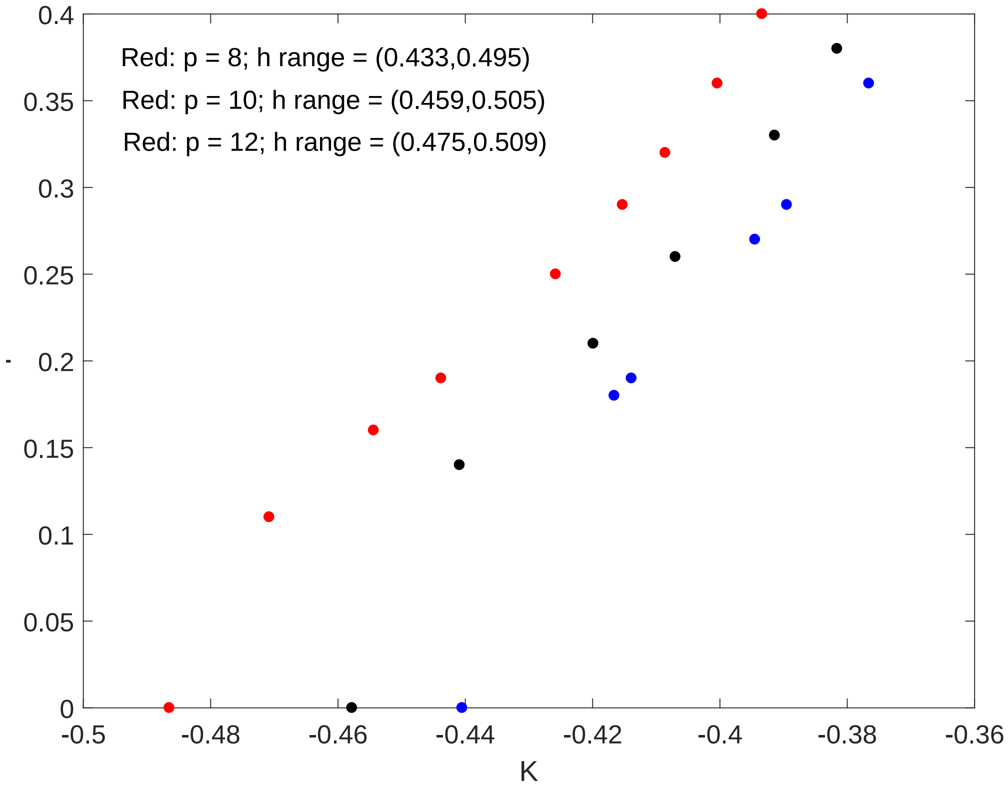
However, first we put in evidence a peculiarity in the phase diagram that was not evident up to now. To this purpose we show again the phase diagram for $p = 8$.

We had considered the diagram for several values of h, spaced 0.2 among them. Now we are going to check a narrower range of h values.


From left: h = 0, h = 0.2, h = 0.4, h = 0.6, h = 0.8, h= 1.0
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
h_c = 0.433
p = 8
T
K
1.2
1
0.8
0.6
0.4
0.2
0
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2



From left: h = 0.4, h = 0.433, h = 0.46, h = 0.48, h = 0.49
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
h_c = 0.433, h* = 0.495
p = 8
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.5
-0.48
-0.46
-0.44
-0.42
-0.4
-0.38
-0.36
K


Red: p = 8; h range = (0.433,0.495)
Red: p = 10; h range = (0.459,0.505)
Red: p = 12; h range = (0.475,0.509)
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.5
-0.48
-0.46
-0.44
-0.42
-0.4
-0.38
-0.36
K

Leaving aside this peculiarity, let us compare the phase transitions lines for the same value of h and the different values of p.

As a hint of what could occur, go back to the expression of the second-order transition line for $h = 0$

$$p\left(\beta \mathrm{e}^{\beta K} - 1\right) + \frac{\beta\left(1 - \mathrm{e}^{2\beta K}\right)}{2} + \frac{\beta\left(1 - e^{\beta K}\right)^2}{2} \tanh^{p-1}\left(\frac{\beta K}{2}\right) = 0\,.$$

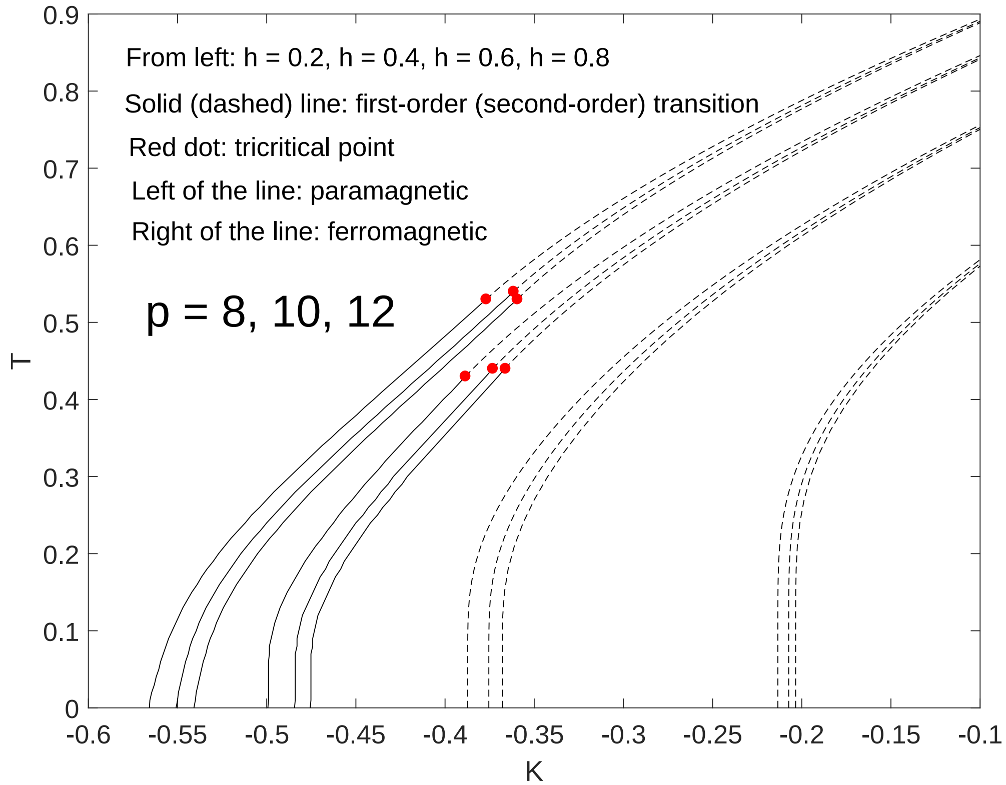
With a power expansion for small K we find

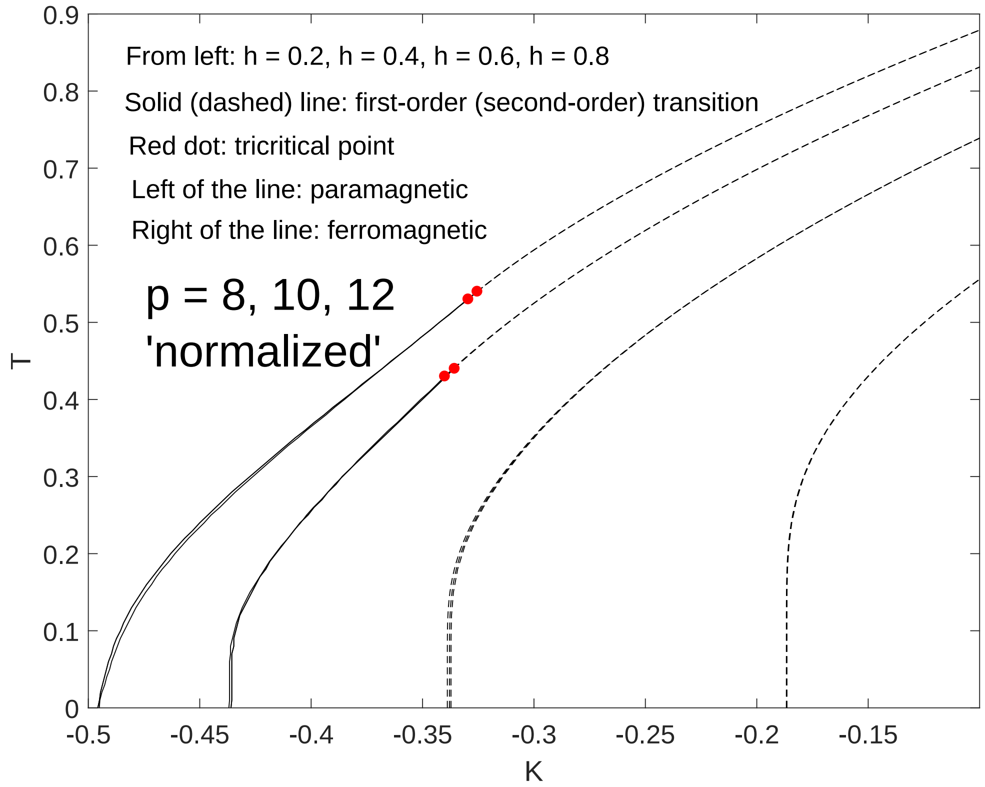
$$T = 1 + \frac{p-1}{p} K\,,$$

that for $p \to \infty$ becomes $T = 1 + K$.

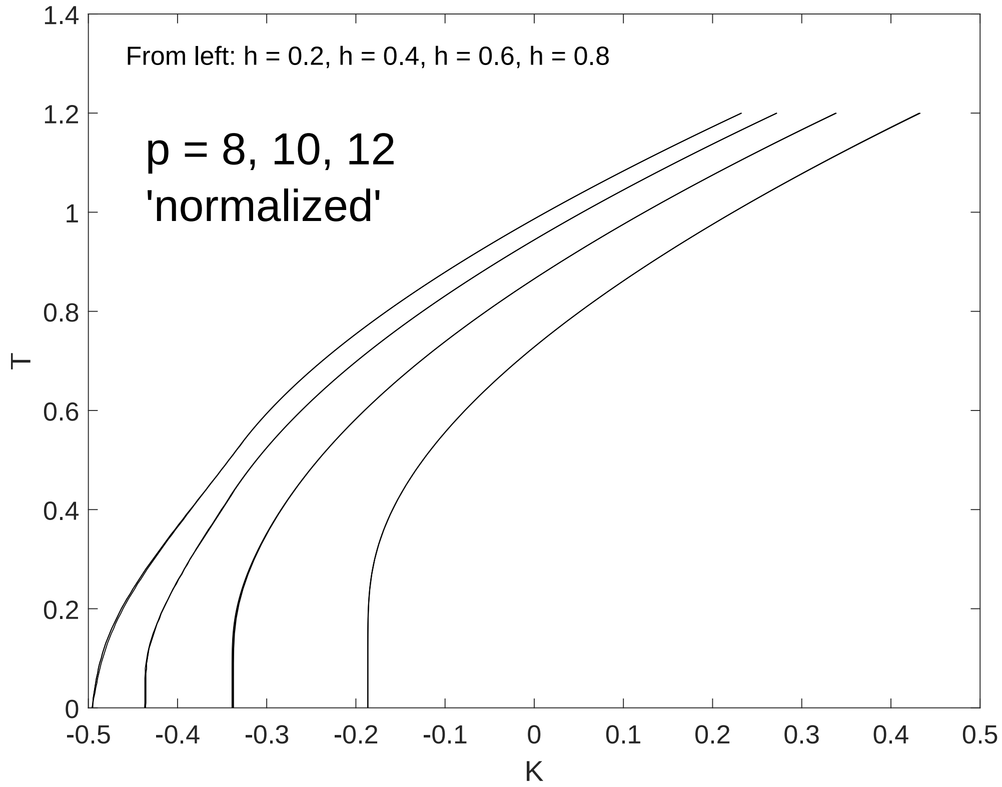
Therefore if for a small K_0 we have a value T_0 for $p = \infty$, then for p we have the same value T_0 for $K = \frac{p}{p-1} K_0$.

This seems to hold for the whole range of negative K interested by the phase transition lines.


From left: h = 0.2, h = 0.4, h = 0.6, h = 0.8
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
p = 8, 10, 12
T
K
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.6
-0.55
-0.5
-0.45
-0.4
-0.35
-0.3
-0.25
-0.2
-0.15
-0.1



From left: h = 0.2, h = 0.4, h = 0.6, h = 0.8
Solid (dashed) line: first-order (second-order) transition
Red dot: tricritical point
Left of the line: paramagnetic
Right of the line: ferromagnetic
p = 8, 10, 12
'normalized'
T
K
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.5
-0.45
-0.4
-0.35
-0.3
-0.25
-0.2
-0.15


From left: h = 0.2, h = 0.4, h = 0.6, h = 0.8
p = 8, 10, 12
'normalized'
T
K
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5

Conclusions

- The structure of first-order and second-order transitions of the classical Nagle-Kardar model persists for sufficiently low transverse fields.
- Instead in the TFIM at $T = 0$ the first-order transition at $K = 0$ becomes, for any small transverse field h a second-order transition at $K = 2h$.
- Strong numerical evidence that already from a relatively small value of p one can obtain the phase diagram of the original model ($p = \infty$).
- The presence of first-order transitions implies ensemble inequivalence.

J. F. Nagle, Phys. Rev. B **2**, 2124 (1970).

J. Roman-Roche et al., Phys. Rev. B **108**, 165130 (2023); J. Roman-Roche, Ph.D. Thesis, Universidad Zaragoza (2024).

N. Defenu et al., Rev. Mod. Phys. **95**, 035002 (2023).

Perspectives

We have considered a 1D system, where with only short-range interactions the system does not exhibit phase transitions at finite temperature. With mean-field (or strong long-range) interactions the critical behaviour is characterized by classical exponents. An interesting situation can arise when a short-range system in, e.g. 2D, which has already phase transitions and its own critical behaviour, is augmented with strong long-range interactions.

It was already proved by Kardar in the classical case, in particular for the 2D Ising model, (Phys. Rev. B **28**, 244 (1983)) that depending on the relative strength of the short-range and the long-range interactions there is a crossover of the critical behaviour. The extension of this study to the quantum case would introduce the quantum fluctuations as a further player in the game.