Introduction to thermodynamics of spin models in the Hamiltonian limit

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Abstract. A didactic description of the thermodynamic properties of classical spin systems is given in terms of their quantum counterpart in the Hamiltonian limit. Emphasis is on the construction of the relevant Hamiltonian, and the calculation of thermal averages is explicitly done in the case of small systems described, in Hamiltonian field theory, by small matrices. The targeted students are those of a graduate statistical physics course

Résumé. On donne une description didactique des propriétés thermodynamiques de systèmes de spins classiques en termes de leur équivalent quantique dans la limite hamiltonienne. On insiste sur la construction de l'hamiltonien et le calcul des moyennes thermiques est effectué explicitement dans le cas de systèmes de petite taille, décrits dans la théorie hamiltonienne des champs par des petites matrices. Le public visé est celui d'étudiants suivant un cours avancés en physique statistique.

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1. Introduction

A rather interesting method for studying thermal fluctuations of $(d+1)$-*dimensional* interacting *classical* degrees of freedom is provided through the corresponding analysis of quantum fluctuations in a *d-dimensional* system of interacting *quantum* degrees of freedom. The correspondence is detailed in the remarkable review of Kogut [1]. It can be understood as a re-wording of the transfer matrix formalism [2] of classical systems in a special limit where the transfer matrix takes a simplified form, the so-called Hamiltonian limit [3]. At the origin of the correspondence, there is the transition amplitude between quantum states in the path integral formulation,

$$\texttt{Amplitude} = \sum_{\texttt{paths}} \exp \frac{i}{\hbar} S[x(t)] \tag{1}$$

where the classical action is a functional of $x(t)$, the time integral of a Lagrangian $S = \int_{t_a}^{t_b} L(x, \dot{x}) dt$. Here we consider the transition amplitude of a point particle (space

dimensionality of the quantum system $d = 0$) for the sake of simplicity. Equation (1) looks a bit similar to the partition function of *something* to be specified,

$$\texttt{P.F.} = \sum_{\texttt{configurations}} \exp(-\beta E\{\texttt{d.o.f.}\}), \tag{2}$$

provided that we change the imaginary argument of the exponential to a real one and we give sense to the degrees of freedom (d.o.f.) and to the sum over their configurations. This transformation is achieved through the definition of an imaginary time, also called Euclidean time,

$$t = -i\tau \tag{3}$$

in terms of which $L(x, \dot{x}) = -H(x, p)$, $p = mx'$, $\dot{x} = dx/dt$ and $x' = dx/d\tau$. The phase factor of equation (1) becomes, with equation (3),

$$\frac{i}{\hbar} S[x(t)] = -\frac{1}{\hbar} \int_{\tau_a}^{\tau_b} H(x, p) d\tau \tag{4}$$

where $H(x, p) = \frac{p^2}{2m} + V(x)$. Equation (1) has a mathematical sense through discretization of the time axis, $t_{i+1} - t_i = \delta = -i\epsilon$, $\epsilon \to 0$, $t_b - t_a = N\delta$, $x_i = x(t_i)$. The action becomes ‡

$$S[x(\tau)] \rightsquigarrow \epsilon \sum_{i=1}^{N-1} \left(\frac{1}{2} m \Big(\frac{x_{i+1} - x_i}{\epsilon} \Big)^2 + V(x_i) \right) \tag{5}$$

and the transition amplitude eventually reads as the partition function of a set of N classical d.o.f. $\{x_i\}$ on a 1-dimensional lattice

$$\begin{aligned} \texttt{Amplitude} &= \int \Big(\prod_i dx_i \Big) \exp(-\hbar^{-1} \sum_i H\{x_i\}) \\ \texttt{P.F.} \qquad &= \sum_{\{x_i\}} \exp(-\beta \sum_i H\{x_i\}). \end{aligned} \tag{6}$$

$H\{x_i\}$ is a classical energy density depending on the set of values taken by the d.o.f., ($-\infty < x_i < +\infty$ if there is no restriction specified in the original quantum problem) and leads after summation to the energy of a configuration appearing in the Boltzmann weight. The role of β (thermal fluctuations) is played by $\hbar^{-1}$ (quantum fluctuations). The classical limit $\hbar \to 0$ where quantum fluctuations are suppressed corresponds to $\beta \to \infty$ in the classical system, i.e. suppression of thermal fluctuations. The correspondence (6) is more generally valid than in the simple case of a point particle. To the statistical physics problem of classical degrees of freedom living in $d + 1$ space dimensions, there corresponds a quantum problem in d dimensions where the fluctuations result from competition between non commutating variables. The partition function of the former problem involves quantum transitions between multi-particle states in the latter formulation and the Hamiltonian limit is the simplest formulation of the quantum problem when only survive transitions between single-particle quantum states.

This approach deserves some attention and might be taught in graduate statistical physics courses. In the following, we remind how the thermodynamic properties of a classical system might be obtained from their quantum counterpart, then we apply the technique to an approximate determination of the critical properties of two-dimensional classical spin models, namely the Ising model and the 3− and 4−state Potts models.

‡ We denote by $S[x(\tau)]$ the functional of a continuous function and $\sum_i H\{x_i\}$ the corresponding sum over a set of discrete variables.

2. Thermodynamics

In the quantum version of the problem, we may define a time evolution operator in terms of which the Feynman kernel is

$$\begin{aligned} K(x_b,t_b|x_a,t_a) &= \langle x_b|\exp(-\frac{i}{\hbar}\hat{\mathbf{H}}(t_b-t_a))|x_a\rangle \\ &= \int \langle x_b|\hat{\mathbf{T}}|x_{N-1}\rangle dx_{N-1}\langle x_{N-1}|\hat{\mathbf{T}}|x_{N-2}\rangle dx_{N-2}\langle x_{N-2}|\dots \\ &\qquad \dots dx_2\langle x_2|\hat{\mathbf{T}}|x_1\rangle dx_1\langle x_1|\hat{\mathbf{T}}|x_a\rangle \\ &= \langle x_b|\hat{\mathbf{T}}^N|x_a\rangle, \end{aligned} \tag{7}$$

where $\hat{\mathbf{T}}$ is the infinitesimal time evolution operator which, in the Euclidean time, becomes the transfer matrix $\hat{\mathbf{T}} = \exp(-\epsilon\hat{\mathbf{H}}/\hbar)$, $\delta = -i\epsilon$. $N\epsilon$ is the length of the system in the supplementary time direction (see Fig. 1). Summing over initial states, when periodic boundary conditions in the time direction are imposed, $x_b = x_a = x_0$, we get the partition function from

$$Z = \int dx_0 K(x_0, -iN\epsilon|x_0,0) = \operatorname{Tr}\hat{\mathbf{T}}^N. \tag{8}$$

The thermodynamic limit $N\to\infty$ ensures projection onto the *ground state*,

$$\hat{\mathbf{T}}^N = t_0^N\Big[|0\rangle\langle 0| + \sum_{\alpha\neq 0}|\alpha\rangle(t_\alpha/t_0)^N\langle\alpha|\Big] \to |0\rangle t_0^N\langle 0| \quad t_0 > t_1 > \dots \tag{9}$$

The partition function is thus determined by the largest eigenvalue t_0 of the transfer matrix,

$$Z \to t_0^N = \mathrm{e}^{-N\epsilon E_0/\hbar}, \tag{10}$$

where E_0 is the ground state energy of the quantum Hamiltonian $\hat{\mathbf{H}}$. The free energy density (i.e. per time slice) follows

$$f = -\lim_{N\to\infty}(N\epsilon)^{-1}\hbar\ln Z \to E_0. \tag{11}$$

The (time) correlation function of some local quantities ϕ_x depending on the classical d.o.f. x, $\langle\phi_{x_i}\phi_{x_{i+j}}\rangle$, is expressed in terms of the transfer matrix through

$$\begin{aligned} \langle\phi_{x_i}\phi_{x_{i+j}}\rangle &= \lim_{N\to\infty} Z^{-1}\sum_{\{x_i\}}\phi_{x_i}\phi_{x_{i+j}}\mathrm{e}^{-\beta E\{x_i\}} \\ &= \lim_{N\to\infty} Z^{-1}\int \langle x_0|\hat{\mathbf{T}}|x_{N-1}\rangle dx_{N-1}\langle x_{N-1}|\dots \\ &\qquad \dots\hat{\mathbf{T}}|x_{i+j}\rangle\phi_{x_{i+j}}dx_{i+j}\langle x_{i+j}|\dots\hat{\mathbf{T}}|x_i\rangle\phi_{x_i}dx_i\langle x_i|\dots \\ &\qquad \dots\hat{\mathbf{T}}|x_1\rangle dx_1\langle x_1|\hat{\mathbf{T}}|x_0\rangle \\ &= \lim_{N\to\infty}\frac{\operatorname{Tr}(\hat{\mathbf{T}}^i\hat{\boldsymbol{\phi}}\hat{\mathbf{T}}^j\hat{\boldsymbol{\phi}}\hat{\mathbf{T}}^{N-i-j})}{\operatorname{Tr}\hat{\mathbf{T}}^N}, \end{aligned} \tag{12}$$

where diagonal operators in the $\{|x_k\rangle\}$ basis have been introduced,

$$\hat{\boldsymbol{\phi}} = \int dx_k|x_k\rangle\phi_{x_k}\langle x_k|. \tag{13}$$

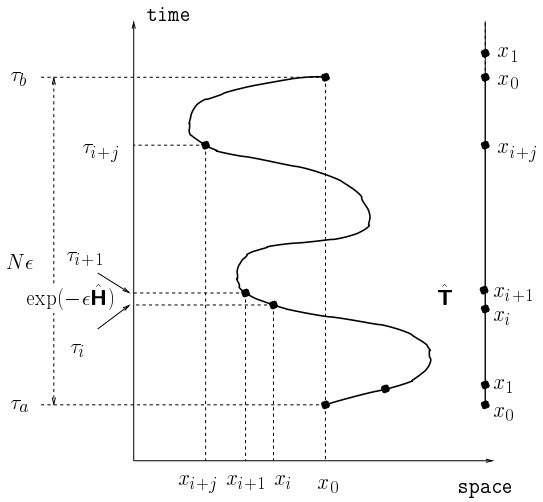

Figure 1. Space-time quantum path and the corresponding classical chain of `d.o.f` x_i. Periodic boundary conditions in time direction are assumed.

Using the eigenstates of the transfer matrix, the correlation function (12) becomes

$$\langle \phi_{x_i} \phi_{x_{i+j}} \rangle = |\langle 0|\hat{\boldsymbol{\phi}}|0\rangle|^2 + \sum_{\alpha \neq 0} |\langle 0|\hat{\boldsymbol{\phi}}|\alpha\rangle|^2 \left(\frac{t_\alpha}{t_0}\right)^j . \tag{14}$$

The connected part of the correlation function, $G_\phi(j)$, is obtained after subtraction of the ground state expectation value, and in the thermodynamic limit it is dominated by the first eigenstate $|\beta_\phi\rangle$ such that the matrix element of $\hat{\boldsymbol{\phi}}$ between this state and the ground state does not vanish,

$$G_\phi(j) \to |\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|^2 \left(\frac{t_\beta}{t_0}\right)^j = |\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|^2 \mathrm{e}^{-j\epsilon\hbar^{-1}(E_\beta - E_0)}. \tag{15}$$

The matrix element in prefactor measures the average of the field squared,

$$\langle \texttt{average field} \rangle = |\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|, \tag{16}$$

and the exponential decay along the time direction allows to define the correlation length in terms of an inverse gap ($\hbar = 1$),

$$\frac{1}{\xi_\phi} = E_\beta - E_0 = \mathtt{gap}_\phi. \tag{17}$$

A challenging problem in critical phenomena is the identification of the universality class of a given model. Due to scaling relations among critical exponents, the knowledge of two of them determines the whole set of exponents (see table 1). From finite size-scaling (FSS) behaviour of the critical densities [4], we expect power law behaviours of local quantities in terms of the finite size L in the space direction,

$$\langle \texttt{Energy density} \rangle \sim L^{-x_\epsilon}, \tag{18}$$

$$\langle \texttt{Order parameter} \rangle \sim L^{-x_\sigma}. \tag{19}$$

These relations may be taken as definitions of the scaling dimensions of the energy and order parameter density, $x_\epsilon = (1-\alpha)/\nu$ and $x_\sigma = \beta/\nu$. The commonly accepted notation for the critical exponents is reminded in table 1. Imagine that we consider a

Table 1. Usual definitions of the critical exponents. The physical quantities are referred to as in the context of a magnetic system.

Quantity	leading singularity	condition	scaling relation
Specific heat	$C(T) \sim \lvert T-T_c\rvert^{-\alpha}$	$h=0$	$\frac{1-\alpha}{\nu} = x_\epsilon$
Magnetization	$M(T) \sim \lvert T-T_c\rvert^{\beta}$	$h=0,\ T<T_c$	$\beta/\nu = x_\sigma$
Susceptibility	$\chi(T) \sim \lvert T-T_c\rvert^{-\gamma}$	$h=0$	$\gamma/\nu = 2-2x_\sigma$
Critical isotherm	$M(h) \sim \lvert h\rvert^{1/\delta}$	$T=T_c$	$\delta = \frac{d-x_\sigma}{x_\sigma}$
Correlation length	$\xi(T) \sim \lvert T-T_c\rvert^{-\nu}$	$h=0$	$\nu = (d-x_\epsilon)^{-1}$
Correlation function	$G(r) \sim r^{-(d-2+\eta)}$	$h=0,\ T=T_c$	$\eta = 2-d+2x$

more general quantum problem in $d-1$-space dimensions. The classical counterpart is defined in d-dimensions (space *and* time) and the susceptibility for example follows from the integration of the correlation function over these d dimensions. Let us write schematically what happens in the case of a translation invariant (in $d-1$ dimensions) matrix element,

$$G_\phi(\mathtt{time}) = |\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|^2 \mathrm{e}^{-\mathtt{gap}_\phi \times \mathtt{time}}, \tag{20}$$

$$\begin{aligned}\chi &= \sum_{\mathtt{space}} \int G_\phi(\mathtt{time})\, d\,\mathtt{time} \\ &\simeq L^{d-1} |\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|^2 \frac{1}{\mathtt{gap}_\phi}.\end{aligned} \tag{21}$$

The matrix element $|\langle 0|\hat{\boldsymbol{\phi}}|\beta_\phi\rangle|$ should scale like L^{-x_ϕ} (see e.g. equations (18) and (19)), hence relation (21) requires that the gap scales according to $\mathtt{gap}_\phi \sim L^{-1}$ in order to restore the usual scaling of the susceptibility $\chi \sim L^{\gamma/\nu}$ with $\gamma/\nu = 2-\eta = d-2x_\phi$ (see table 1). Note that the gap being an inverse correlation length, its scaling inversely proportional to the typical linear size of the system logically means that the correlation length at criticality is locked at that size.

The scaling of the gap is more constrained in $2d$ where rather powerful techniques apply. Conformal invariance indeed provides quite efficient methods for the determination of critical exponents of two-dimensional critical systems [5]. The cylinder geometry is relevant in the study of quantum chains, since such a chain with periodic boundary conditions in the space direction just corresponds to an infinitely long classical cylinder ($1+1$ dimensions) of complex coordinates $w = \mathtt{time} + i \times \mathtt{space}$ (here, Euclidean time is assumed). This former geometry follows from the infinite two-dimensional plane $z = r\mathrm{e}^{i\theta}$ through the standard logarithmic mapping $w(z) = \frac{L}{2\pi} \ln z$ and, at the critical point, the correlation functions transform according to conformal covariance, leading along the cylinder to [6]

$$G_\phi(\mathtt{time}) = \left(\frac{2\pi}{L}\right)^{2x_\phi} \mathrm{e}^{-\frac{2\pi}{L} x_\phi \times \mathtt{time}}. \tag{22}$$

From comparison with equation (20), the critical correlation length amplitude appears universal and its value related to the corresponding critical exponent through the simple relation

$$\mathtt{gap}_\phi = \frac{2\pi}{L} x_\phi. \tag{23}$$

The matrix elements are also predicted by conformal invariance and follow from equation (22),

$$|\langle 0|\hat{\phi}|\beta\rangle| = \left(\frac{2\pi}{L}\right)^{x_\phi}. \tag{24}$$

A prescription before using any conformal invariance result concerns the scaling of the whole spectrum. Multiplying the Hamiltonian by an arbitrary number of course changes the scale of the spectrum. Gap scaling from equation (23) requires to fix the normalization in such a way that the sound velocity is unity [7]. The sound velocity might be defined in the long-wavelength limit, `sound velocity` $= \Delta E/\Delta k$, where ΔE is for instance measured by gaps in the bottom of the spectrum and $\Delta k = 2\pi/L$ is given by the quantization step of wave vectors.

3. Quantum Ising chain

The two-dimensional Ising model is often used as the paradigmatic illustration of second-order phase transitions. It is one of the most simple non trivial models and in the following we will show how its quantum counterpart, the quantum Ising chain in a transverse field, is built.

3.1. The Hamiltonian limit

Let us first consider a ladder of classical Ising spins $s_{i,j} = \pm 1$, $-\infty < i < +\infty$, and $j = 1, 2$ (see figure 2). The nearest neighbour interactions are denoted as $K_s = \beta J_s$ in the space (j) direction and $K_t = \beta J_t$ in the time (i) direction. The energy of a

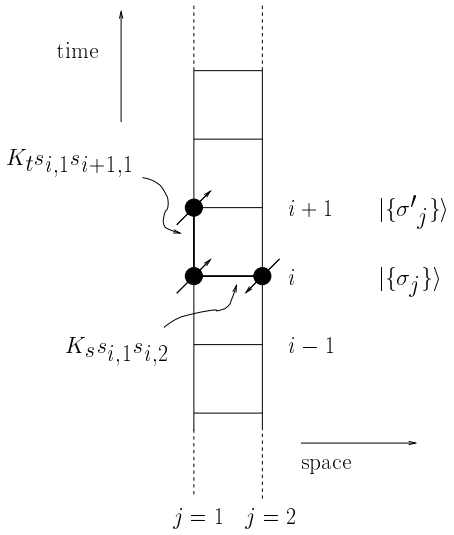

Figure 2. Infinite ladder of Ising spins.

configuration is a sum over time slices,

$$-\beta E\{s_{i,j}\} = \sum_i (K_s s_{i,1}s_{i,2} + K_t(s_{i,1}s_{i+1,1} + s_{i,2}s_{i+1,2})), \tag{25}$$

and the partition function reads as

$$Z = \operatorname*{Tr}_{\{s_{i,j}\}} \prod_i \mathrm{e}^{K_s s_{i,1}s_{i,2} + K_t(s_{i,1}s_{i+1,1} + s_{i,2}s_{i+1,2})} = \operatorname*{Tr}_{\{s_{i,j}\}} \prod_i T_{i,i+1}, \tag{26}$$

where $T_{i,i+1}$ is an element of some transfer matrix between row states $|\{\sigma_j\}\rangle = |s_{i,1}, s_{i,2}\rangle$ and $|\{\sigma'_j\}\rangle = |s_{i+1,1}, s_{i+1,2}\rangle$ at rows i and $i+1$ (see figure 2),

$$T_{i,i+1} = \langle\{\sigma'_j\}|\hat{\mathbf{T}}|\{\sigma_j\}\rangle. \tag{27}$$

$\hat{\mathbf{T}}$ is a 4×4 matrix, since the two spins σ_1, σ_2 have four different configurations. The space coupling term is diagonal, $\delta_{\{\sigma_j\},\{\sigma'_j\}} \times \exp(K_s\sigma_1\sigma_2)$,

$$\begin{array}{c|c|cccc} \sigma_1,\sigma_2 \diagdown \sigma'_1,\sigma'_2 & & |\uparrow,\uparrow\rangle & |\uparrow,\downarrow\rangle & |\downarrow,\uparrow\rangle & |\downarrow,\downarrow\rangle \\ \hline \langle\uparrow,\uparrow| & & \mathrm{e}^{K_s} & 0 & 0 & 0 \\ \langle\uparrow,\downarrow| & & 0 & \mathrm{e}^{-K_s} & 0 & 0 \\ \langle\downarrow,\uparrow| & & 0 & 0 & \mathrm{e}^{-K_s} & 0 \\ \langle\downarrow,\downarrow| & & 0 & 0 & 0 & \mathrm{e}^{K_s} \end{array}, \tag{28}$$

while a non-diagonal contribution due to possible spin flips in the time direction, $\exp[K_t(\sigma_1\sigma'_1 + \sigma_2\sigma'_2)]$, leads to the following matrix

$$\begin{array}{c|c|cccc} \sigma_1,\sigma_2 \diagdown \sigma'_1,\sigma'_2 & & |\uparrow,\uparrow\rangle & |\uparrow,\downarrow\rangle & |\downarrow,\uparrow\rangle & |\downarrow,\downarrow\rangle \\ \hline \langle\uparrow,\uparrow| & & \mathrm{e}^{2K_t} & 1 & 1 & \mathrm{e}^{-2K_t} \\ \langle\uparrow,\downarrow| & & 1 & \mathrm{e}^{2K_t} & \mathrm{e}^{-2K_t} & 1 \\ \langle\downarrow,\uparrow| & & 1 & \mathrm{e}^{-2K_t} & \mathrm{e}^{2K_t} & 1 \\ \langle\downarrow,\downarrow| & & \mathrm{e}^{-2K_t} & 1 & 1 & \mathrm{e}^{2K_t} \end{array}. \tag{29}$$

The transfer matrix $\hat{\mathbf{T}}$ should be identified through its matrix elements. For the diagonal term, we introduce *diagonal operators* in the $|\{\sigma_j\}\rangle$ basis, namely

$$\hat{\boldsymbol{\sigma}}_z(1) = \sum_{\sigma_1,\sigma_2} |\sigma_1,\sigma_2\rangle\sigma_1\langle\sigma_1,\sigma_2|, \quad [\hat{\boldsymbol{\sigma}}_z(1)] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_1 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_2, \tag{30}$$

$$\hat{\boldsymbol{\sigma}}_z(2) = \sum_{\sigma_1,\sigma_2} |\sigma_1,\sigma_2\rangle\sigma_2\langle\sigma_1,\sigma_2|, \quad [\hat{\boldsymbol{\sigma}}_z(2)] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_1 \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_2, \tag{31}$$

where $(\hat{\mathbf{1}})_j$ and $(\hat{\boldsymbol{\sigma}}_z)_j$ represent the 2×2 identity or Pauli matrix acting only on variables σ_j at site j. The matrix in equation (28) is identified to that of the operator

$$\exp(K_s\hat{\boldsymbol{\sigma}}_z(1)\hat{\boldsymbol{\sigma}}_z(2)). \tag{32}$$

For the flipping term, we introduce *transition operators*

$$\hat{\boldsymbol{\sigma}}_x(1)|\sigma_1,\sigma_2\rangle = |-\sigma_1,\sigma_2\rangle, \quad [\hat{\boldsymbol{\sigma}}_x(1)] = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_1 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_2, \tag{33}$$

$$\hat{\boldsymbol{\sigma}}_x(2)|\sigma_1,\sigma_2\rangle = |\sigma_1,-\sigma_2\rangle, \quad [\hat{\boldsymbol{\sigma}}_x(2)] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_1 \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_2, \tag{34}$$

and since $\hat{\boldsymbol{\sigma}}_x^2(j) = \hat{\mathbf{1}}$, we have, for any value of $K_t^\star$, the useful identity

$$\exp[K_t^\star \hat{\boldsymbol{\sigma}}_x(j)] = \hat{\mathbf{1}} \cosh K_t^\star + \hat{\boldsymbol{\sigma}}_x(j) \sinh K_t^\star, \tag{35}$$

so that the matrix in equation (29) is identified to that of the operator $\mathrm{e}^{K_t^\star(\hat{\boldsymbol{\sigma}}_x(1)+\hat{\boldsymbol{\sigma}}_x(2))}$,

$$\begin{pmatrix} \cosh^2 K_t^\star & \cosh K_t^\star \sinh K_t^\star & \cosh K_t^\star \sinh K_t^\star & \sinh^2 K_t^\star \\ \cosh K_t^\star \sinh K_t^\star & \cosh^2 K_t^\star & \sinh^2 K_t^\star & \cosh K_t^\star \sinh K_t^\star \\ \cosh K_t^\star \sinh K_t^\star & \sinh^2 K_t^\star & \cosh^2 K_t^\star & \cosh K_t^\star \sinh K_t^\star \\ \sinh^2 K_t^\star & \cosh K_t^\star \sinh K_t^\star & \cosh K_t^\star \sinh K_t^\star & \cosh^2 K_t^\star \end{pmatrix}, \tag{36}$$

(up to a prefactor which only shifts the free energy by a constant) provided that we demand

$$\tanh K_t^\star = \mathrm{e}^{-2K_t}. \tag{37}$$

This relation is equivalent to the usual duality relation

$$\sinh 2K_t \sinh 2K_t^\star = 1. \tag{38}$$

The transfer matrix eventually follows (we use $\mathrm{e}^{\mathbf{A}+\mathbf{B}} = \mathrm{e}^{\mathbf{A}}\mathrm{e}^{\mathbf{B}}\mathrm{e}^{-[\mathbf{A},\mathbf{B}]/2}\ldots$ and already take into account the simplification due to the extreme anisotropic limit which eliminates all correction terms)

$$\hat{\mathbf{T}} = \exp(K_s \hat{\boldsymbol{\sigma}}_z(1)\hat{\boldsymbol{\sigma}}_z(2)) \times \exp(K_t^\star(\hat{\boldsymbol{\sigma}}_x(1) + \hat{\boldsymbol{\sigma}}_x(2)). \tag{39}$$

The multiple spin flip terms appear in the expansion of the exponential through product of terms like in equation (35). The generalization to a lattice of width L in the space direction (we choose now for the rest of the paper periodic boundary conditions $\hat{\boldsymbol{\sigma}}_{x,z}(L+1) = \hat{\boldsymbol{\sigma}}_{x,z}(1)$ in space direction) is straightforward, summing over $j = 1, L$,

$$\hat{\mathbf{T}} = \exp(K_s \sum_{j=1}^{L} \hat{\boldsymbol{\sigma}}_z(j)\hat{\boldsymbol{\sigma}}_z(j+1)) \times \exp(K_t^\star \sum_{j=1}^{L} \hat{\boldsymbol{\sigma}}_x(j)). \tag{40}$$

The transfer matrix has a complicated structure, since arbitrary large numbers of single spin transitions may simultaneously occur and the matrix representation of $\hat{\mathbf{T}}$ is expected to be dense. It may be considerably simplified in the extreme anisotropic limit also called Hamiltonian limit, since then only single spin transitions survive and $\hat{\mathbf{H}}$ is a sparser matrix. Remember that the relation between the transfer matrix and the Hamiltonian involves the lattice spacing ϵ in the time direction which tends to zero, $\hat{\mathbf{T}} = \exp(-\epsilon\hat{\mathbf{H}}) = \hat{\mathbf{1}} - \epsilon\hat{\mathbf{H}} + O(\epsilon^2)$. A simple limit of $\hat{\mathbf{T}}$ in equation (40) is obtained when $K_s \to 0$, $K_t \to \infty$ (or $K_t^\star \to 0$), with $K_s/K_t^\star = \lambda = O(1)$, and in order to avoid unnecessary constants, we may set $\epsilon = 2K_t^\star$ § to get

$$\hat{\mathbf{H}} = -\frac{1}{2}\lambda \sum_{j=1}^{L} \hat{\boldsymbol{\sigma}}_z(j)\hat{\boldsymbol{\sigma}}_z(j+1)) - \frac{1}{2}\sum_{j=1}^{L} \hat{\boldsymbol{\sigma}}_x(j). \tag{41}$$

The critical line of the two-dimensional anisotropic classical system, obtained through duality i.e. when the relation $\sinh 2K_s \sinh 2K_t = 1$ is fulfilled, is equivalent in the extreme anisotropic limit to $2K_s(2K_t^\star)^{-1} = \lambda_c = 1$ when equation (38) is also used. Fluctuations in the ground state structure have their origin in the competition

§ The normalization with a factor 2 ensures a sound velocity equal to 1 (i.e. a linear dispersion relation at long wavelength with slope unity) and is necessary in order to compare later with conformal invariance predictions (see discussion).

between two non-commuting terms in the Hamiltonian. In expression (41), the term $-\lambda\hat{\boldsymbol{\sigma}}_z(j)\hat{\boldsymbol{\sigma}}_z(j+1)$ acts like a ferromagnetic interaction which reinforces order in the z-direction (order parameter) in the chain, while $\hat{\boldsymbol{\sigma}}_x(j)$ appears as a disordering flipping term. When $\lambda > 1$, the ordering term dominates and we expect ferromagnetic z-order in the ground state, while the disordered phase corresponds to a dominant role of the flipping term when $\lambda < 1$.

3.2. The symmetries of the model

The classical model exhibits the Z_2 symmetry (invariance under global change $+1 \longleftrightarrow -1$ on each site). In the quantum case we expect a similar property ‖ $|\uparrow,\downarrow,\uparrow,\ldots,\uparrow\rangle_z \longleftrightarrow |\downarrow,\uparrow,\downarrow,\ldots,\downarrow\rangle_z$. This property has an algebraic manifestation through the commutator

$$[\hat{\mathbf{H}},\hat{\mathbf{P}}] = 0, \quad \hat{\mathbf{P}} = \prod_{j=1}^{L} \hat{\boldsymbol{\sigma}}_x(j). \tag{42}$$

The eigenstates of $\hat{\mathbf{H}}$ may then be classified according to their parity, $P = \pm 1$, $\hat{\mathbf{P}}|\texttt{even state}\rangle = +1|\texttt{even state}\rangle$ and $\hat{\mathbf{P}}|\texttt{odd state}\rangle = -1|\texttt{odd state}\rangle$ and an obvious consequence is that $\hat{\mathbf{H}}$ has vanishing matrix elements between states of different parities. More generally, for any *even* operator $\hat{\mathbf{E}}$ such that $\hat{\mathbf{E}}\hat{\mathbf{P}} = \hat{\mathbf{P}}\hat{\mathbf{E}}$, the only possibly non vanishing matrix elements of $\hat{\mathbf{E}}$ are between states of the same parity while *odd* operators satisfying $\hat{\mathbf{O}}\hat{\mathbf{P}} = -\hat{\mathbf{P}}\hat{\mathbf{O}}$ have surviving matrix elements between states of opposite parities. The ground state of the system is expected to be even (it is of the symmetry of the Hamiltonian itself), so that a measure of local order in the system is given in agreement with equation (16) by

$$\langle\texttt{Order parameter}\rangle = |\langle\texttt{Lowest odd state}|\hat{\boldsymbol{\sigma}}_z(j)|\texttt{Gnd}\rangle|. \tag{43}$$

A similar definition of the energy density may be given by inserting terms appearing into the Hamiltonian inside states of the same parity, e.g.

$$\langle\texttt{Energy density}\rangle = |\langle\texttt{1st excited even state}|\hat{\boldsymbol{\sigma}}_x(j)|\texttt{Gnd}\rangle|. \tag{44}$$

Matrix elements of $\hat{\boldsymbol{\sigma}}_z(j)\hat{\boldsymbol{\sigma}}_z(j+1)$ might have been chosen as well. The reason for being mainly interested in the bottom of the spectrum (see figure 3) lies in the fact that the quantum phase transition takes place at zero temperature. Together with the eigenstates already mentioned, we define the state $|\texttt{sound velocity}\rangle$ and the corresponding relation which fixes the value of the sound velocity,

$$E_{v_s} - E_{\texttt{Order}} = \frac{2\pi}{L} v_s. \tag{45}$$

If the normalization is not properly chosen, or if the sound velocity is not known, equation (23) should be replaced by

$$\texttt{gap}_\phi = \frac{2\pi}{L} v_s x_\phi \tag{46}$$

and v_s obtained by the equation above. In the case of the quantum Ising model, the Hamiltonian (41) is conveniently normalized and $v_s = 1$ [8].

‖ For simplicity, we use a short notation $|\uparrow,\downarrow,\uparrow,\ldots,\uparrow\rangle$ for $|\uparrow_1\rangle \otimes |\downarrow_2\rangle \otimes |\uparrow_3\rangle \otimes \ldots \otimes |\uparrow_L\rangle$.

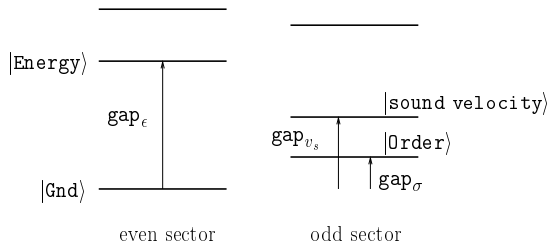

Figure 3. Structure of the bottom of the spectrum.

3.3. Small Chains

A quantum chain of length L corresponds to an infinitely long ladder or strip of classical spins $s_{i,j}$. In the case of a chain of 2 spins with periodic boundary conditions (the classical counterpart is thus a cylinder), the Hamiltonian may be written

$$-2\hat{\mathbf{H}} = \lambda\hat{\boldsymbol{\sigma}}_z(1)\hat{\boldsymbol{\sigma}}_z(2) + \lambda\hat{\boldsymbol{\sigma}}_z(2)\hat{\boldsymbol{\sigma}}_z(1) + \hat{\boldsymbol{\sigma}}_x(1) + \hat{\boldsymbol{\sigma}}_x(2). \tag{47}$$

The construction of the matrix of $\hat{\mathbf{H}}$ is easy,

$$[-2\hat{\mathbf{H}}] = \begin{pmatrix} 2\lambda & 1 & 1 & 0 \\ 1 & -2\lambda & 0 & 1 \\ 1 & 0 & -2\lambda & 1 \\ 0 & 1 & 1 & 2\lambda \end{pmatrix} \begin{matrix} |\uparrow,\uparrow\rangle_z \\ |\uparrow,\downarrow\rangle_z \\ |\downarrow,\uparrow\rangle_z \\ |\downarrow,\downarrow\rangle_z \end{matrix} \tag{48}$$

but it is not written here in the simplest way. Due to the parity property of $\hat{\mathbf{H}}$, it is easier to write the 4×4 matrix in the basis of $\hat{\boldsymbol{\sigma}}_x$-eigenstates, where it is block diagonal. In *the basis* $\{|\uparrow,\uparrow\rangle_x, |\downarrow,\downarrow\rangle_x, |\uparrow,\downarrow\rangle_x, |\downarrow,\uparrow\rangle_x\}$, we have

$$[-2\hat{\mathbf{H}}] = \left(\begin{array}{cc|cc} 2 & 2\lambda & 0 & \\ 2\lambda & -2 & & \\ \hline 0 & & 0 & 2\lambda \\ & & 2\lambda & 0 \end{array}\right) \begin{matrix} |\uparrow,\uparrow\rangle_x \\ |\downarrow,\downarrow\rangle_x \\ |\uparrow,\downarrow\rangle_x \\ |\downarrow,\uparrow\rangle_x \end{matrix} \tag{49}$$

In the even sector at the critical coupling $\lambda_c = 1$, the eigenvalues of $\hat{\mathbf{H}}$ are $E_{\mathtt{Gnd}} = -\sqrt{2}$ and $E_{\mathtt{Energy}} = +\sqrt{2}$. The ground state $|\mathtt{Gnd}\rangle = a^{\uparrow\uparrow}_{\mathtt{Gnd}}|\uparrow,\uparrow\rangle_x + a^{\downarrow\downarrow}_{\mathtt{Gnd}}|\downarrow,\downarrow\rangle_x$ has normalized components $a^{\uparrow\uparrow}_{\mathtt{Gnd}} = 0.924$ and $a^{\downarrow\downarrow}_{\mathtt{Gnd}} = 0.383$ while the *energy* excited state is given by $|\mathtt{Energy}\rangle = a^{\uparrow\uparrow}_{\mathtt{Energy}}|\uparrow,\uparrow\rangle_x + a^{\downarrow\downarrow}_{\mathtt{Energy}}|\downarrow,\downarrow\rangle_x$ with $a^{\uparrow\uparrow}_{\mathtt{Energy}} = 0.383$ and $a^{\downarrow\downarrow}_{\mathtt{Energy}} = -0.924$. The energy matrix element follows,

$$\begin{aligned} \langle\mathtt{Energy\ density}\rangle &= |\langle\mathtt{Energy}|\hat{\boldsymbol{\sigma}}_x(1)|\mathtt{Gnd}\rangle| \\ &= |a^{\uparrow\uparrow}_{\mathtt{Energy}}a^{\uparrow\uparrow}_{\mathtt{Gnd}} - a^{\downarrow\downarrow}_{\mathtt{Energy}}a^{\downarrow\downarrow}_{\mathtt{Gnd}}| \\ &= 0.707. \end{aligned} \tag{50}$$

In the odd sector, the lowest eigenvalue is $E_{\mathtt{Order}} = -1$ and the corresponding eigenvector $|\mathtt{Order}\rangle = a^{\uparrow\downarrow}_{\mathtt{Order}}|\uparrow,\downarrow\rangle_x + a^{\downarrow\uparrow}_{\mathtt{Order}}|\downarrow,\uparrow\rangle_x$ has components $a^{\uparrow\downarrow}_{\mathtt{Order}} = a^{\downarrow\uparrow}_{\mathtt{Order}} = 0.707$. The order parameter matrix element follows,

$$\begin{aligned} \langle\mathtt{Order\ parameter}\rangle &= |\langle\mathtt{Order}|\hat{\boldsymbol{\sigma}}_z(1)|\mathtt{Gnd}\rangle| \\ &= |a^{\uparrow\downarrow}_{\mathtt{Order}}a^{\downarrow\downarrow}_{\mathtt{Gnd}} + a^{\downarrow\uparrow}_{\mathtt{Order}}a^{\uparrow\uparrow}_{\mathtt{Gnd}}| \\ &= 0.924. \end{aligned} \tag{51}$$

Table 2. Values of the physical properties of small quantum Ising chains.

L	$E_{\texttt{Gnd}}$	$E_{\texttt{Energy}}$	$E_{\texttt{Order}}$	$\langle$`Energy density`$\rangle$	$\langle$`Order parameter`$\rangle$
2	-1.414	$+1.414$	-1.000	0.707	0.924
3	-2.000	0.000	-1.732	0.577	0.880
4	-2.613	-1.082	-2.414	0.462	0.848

In the case of a chain of 3 spins with periodic boundary conditions, we have in the basis of σ_x eigenstates

$$[-2\hat{\mathbf{H}}] = \left(\begin{array}{cccc|cccc} 3 & \lambda & \lambda & \lambda & & & & \\ \lambda & -1 & \lambda & \lambda & & & & \\ \lambda & \lambda & -1 & \lambda & & & & \\ \lambda & \lambda & \lambda & -1 & & & & \\ \hline & & & & -3 & \lambda & \lambda & \lambda \\ & & & & \lambda & 1 & \lambda & \lambda \\ & & & & \lambda & \lambda & 1 & \lambda \\ & & & & \lambda & \lambda & \lambda & 1 \end{array}\right) \begin{array}{l} |\uparrow,\uparrow,\uparrow\rangle_x \\ |\downarrow,\downarrow,\uparrow\rangle_x \\ |\uparrow,\downarrow,\downarrow\rangle_x \\ |\downarrow,\uparrow,\downarrow\rangle_x \\ |\downarrow,\downarrow,\downarrow\rangle_x \\ |\uparrow,\uparrow,\downarrow\rangle_x \\ |\downarrow,\uparrow,\uparrow\rangle_x \\ |\uparrow,\downarrow,\uparrow\rangle_x \end{array} \tag{52}$$

The relevant energy levels and corresponding matrix elements for three small sizes are collected in table 2. Use will be made of these results to get approximate values of the critical exponents in the discussion in section 5.

4. Quantum Potts chain

The Potts model generalizes the Ising model. The sites are occupied by Potts variables (abusively called spins) with q different states, $n_{i,j} = 0, 1, \ldots q-1$, and bonds between nearest neighbour sites may have two different energy levels, depending on the relative states of the site variables, e.g. $-J(q\delta_{n,n'} - 1)$.

4.1. Hamiltonian limit

We follow the same steps as in the case of the Ising model [9, 10]. The energy of a configuration is written as a sum over time slices,

$$-\beta E\{n_{i,j}\} = \sum_i \left[K_s \sum_{j=1}^{L} (q\delta_{n_{i,j},n_{i,j+1}} - 1) + K_t \sum_{j=1}^{L} (q\delta_{n_{i,j},n_{i+1,j}} - 1) \right], \tag{53}$$

where the fact that interactions are limited to nearest neighbours allows a factorized partition function $Z = \mathrm{Tr}_{\{n_{i,j}\}} \prod_i T_{i,i+1}$ with matrix elements between row states $|\{\nu_j\}\rangle = |n_{i,1}, n_{i,2}, \ldots n_{i,L}\rangle$ and $|\{\nu'_j\}\rangle = |n_{i+1,1}, n_{i+1,2}, \ldots n_{i+1,L}\rangle$ at time indexes i and $i+1$,

$$T_{i,i+1} = \langle\{\nu'_j\}|\hat{\mathbf{T}}|\{\nu_j\}\rangle. \tag{54}$$

Now $\hat{\mathbf{T}}$ is a $q^L \times q^L$ matrix (each of the L spins $n_{i,j}$ have q different possible states). As in the case of the Ising model, the space coupling term is diagonal, $\delta_{\{\nu_j\},\{\nu'_j\}} \times \exp(qK_s \sum_k (\delta_{n_{i,k},n_{i,k+1}} - 1))$. Its description in $\hat{\mathbf{T}}$ requires the introduction of a combination of diagonal operators in the basis $|\{\nu_j\}\rangle$, the matrix element of which reproduces the Kronecker delta. For that purpose, we define state vector

$|\nu_1\rangle \otimes |\nu_2\rangle \otimes \ldots \otimes |\nu_L\rangle \equiv |\nu_1, \nu_2, \ldots, \nu_L\rangle$ and the corresponding diagonal operators $\hat{\mathbf{C}}_k$ and $\hat{\mathbf{C}}_k^\dagger$ such that (in this section, we stay close to the notations of Ref. [11])

$$\begin{aligned}\hat{\mathbf{C}}_k|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle &\equiv \mathrm{e}^{2i\pi\nu_k/q}|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle,\\ \hat{\mathbf{C}}_k^\dagger|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle &\equiv \mathrm{e}^{-2i\pi\nu_k/q}|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle. \end{aligned} \tag{55}$$

Due to the property

$$\frac{1}{q}\sum_{p=0}^{q-1} \mathrm{e}^{-2ip\pi(\nu_k-\nu_l)/q} = \delta_{\nu_k,\nu_l}$$

we may write the Kronecker delta as the diagonal matrix element

$$\delta_{\nu_k,\nu_l} = \langle\{\nu_j\}|\frac{1}{q}\sum_{p=0}^{q-1}(\hat{\mathbf{C}}_k^\dagger\hat{\mathbf{C}}_l)^p|\{\nu_j\}\rangle. \tag{56}$$

and thus the space contribution to the transfer matrix follows

$$\exp\left(K_s\sum_{j=1}^{L}\sum_{p=1}^{q-1}(\hat{\mathbf{C}}_j^\dagger\hat{\mathbf{C}}_{j+1})^p\right) \tag{57}$$

where the term $p = 0$ is subtracted, since it compensates the -1 in the definition of the pair energy in equation (53). For the time contribution, it is necessary to introduce flipping operators and we define

$$\begin{aligned}\hat{\mathbf{R}}_k|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle &\equiv |\nu_1, \nu_2, \ldots, \nu_k + 1, \ldots, \nu_L\rangle,\\ \hat{\mathbf{R}}_k^\dagger|\nu_1, \nu_2, \ldots, \nu_k, \ldots, \nu_L\rangle &\equiv |\nu_1, \nu_2, \ldots, \nu_k - 1, \ldots, \nu_L\rangle, \end{aligned} \tag{58}$$

where periodicity in space state is assumed, $|\nu + q\rangle = |\nu\rangle$. The matrix representation of these operators is the following

$$[\hat{\mathbf{C}}_j] = \hat{\mathbf{1}}\otimes\hat{\mathbf{1}}\otimes\ldots\otimes\begin{pmatrix} 1 & 0 & 0 & \ldots & 0\\ 0 & \mathrm{e}^{2i\pi/q} & 0 & \ldots & 0\\ \vdots & 0 & \mathrm{e}^{4i\pi/q} & \ddots & \vdots\\ 0 & \vdots & \ddots & \ddots & 0\\ 0 & 0 & \ldots & 0 & \mathrm{e}^{2i\pi(q-1)/q}\end{pmatrix}_j \ldots\otimes\hat{\mathbf{1}}, \tag{59}$$

$$[\hat{\mathbf{R}}_j] = \hat{\mathbf{1}}\otimes\hat{\mathbf{1}}\otimes\ldots\otimes\begin{pmatrix} 0 & 0 & \ldots & 0 & 1\\ 1 & 0 & \ldots & 0 & 0\\ 0 & 1 & \ddots & \vdots & \vdots\\ \vdots & \ddots & 1 & 0 & 0\\ 0 & \ldots & 0 & 1 & 0\end{pmatrix}_j \ldots\otimes\hat{\mathbf{1}}. \tag{60}$$

They commute on different sites and obey the following algebra on a given site $\hat{\mathbf{R}}_j\hat{\mathbf{C}}_j = \mathrm{e}^{-2i\pi/q}\hat{\mathbf{C}}_j\hat{\mathbf{R}}_j$, $\hat{\mathbf{R}}_j^\dagger\hat{\mathbf{C}}_j = \mathrm{e}^{2i\pi/q}\hat{\mathbf{C}}_j\hat{\mathbf{R}}_j^\dagger$, $\hat{\mathbf{R}}_j\hat{\mathbf{C}}_j^\dagger = \mathrm{e}^{2i\pi/q}\hat{\mathbf{C}}_j^\dagger\hat{\mathbf{R}}_j$, $\hat{\mathbf{R}}_j^\dagger\hat{\mathbf{C}}_j^\dagger = \mathrm{e}^{-2i\pi/q}\hat{\mathbf{C}}_j^\dagger\hat{\mathbf{R}}_j^\dagger$, $\hat{\mathbf{C}}_j^q = \hat{\mathbf{R}}_j^q = \hat{\mathbf{1}}$. Temporarily forgetting about the site index, diagonalization of $\hat{\mathbf{R}}$ leads to

$$\hat{\mathbf{R}}|r\rangle = \mathrm{e}^{2ir\pi/q}|r\rangle, \quad |r\rangle = q^{-1/2}\sum_{\nu=0}^{q-1}\mathrm{e}^{-(2ir\pi/q)\nu}|\nu\rangle.$$

It follows that the operator $\hat{\mathbf{\Theta}} \equiv \frac{1}{q}\sum_{p=0}^{q-1}\hat{\mathbf{R}}^p$ has the property $\hat{\mathbf{\Theta}}|r\rangle = \delta_{r,0}|r\rangle$ (it is equal the projector on the "zero eigenstate" of $\hat{\mathbf{R}}$, $\hat{\mathbf{\Theta}} = |r=0\rangle\langle r=0|$, and so $\langle\{\nu'_j\}|\hat{\mathbf{\Theta}}|\{\nu_j\}\rangle = 1/q$ for any pair of states $|\{\nu_j\}\rangle$ and $|\{\nu'_j\}\rangle$) which enables to write

$$\exp(qK_t^\star\hat{\mathbf{\Theta}}_j) = \hat{\mathbf{1}} + \hat{\mathbf{\Theta}}_j(\mathrm{e}^{qK_t^\star} - 1) \tag{61}$$

for arbitrary value of $K_t^\star$. The time contributions, $\mathrm{e}^{K_t(q\delta_{\nu_j,\nu'_j}-1)}$, which can take values $\mathrm{e}^{K_t(q-1)}$ if $\nu'_j = \nu_j$ and e^{-K_t} otherwise, are obtained from matrix elements of terms $\exp(qK_t^\star\hat{\mathbf{\Theta}}_j)$ provided that $K_t^\star$ satisfies the duality relation

$$(\mathrm{e}^{qK_t} - 1)(\mathrm{e}^{qK_t^\star} - 1) = q. \tag{62}$$

The transfer matrix eventually reads as

$$\hat{\mathbf{T}} = \exp\left(K_s\sum_{j=1}^{L}\sum_{p=1}^{q-1}(\hat{\mathbf{C}}_j^\dagger\hat{\mathbf{C}}_{j+1})^p\right) \times \exp\left(K_t^\star\sum_{j=1}^{L}\sum_{p=1}^{q-1}\hat{\mathbf{R}}_j^p\right). \tag{63}$$

We have shifted the sum in the last term, starting from $p = 1$ which only changes the transfer matrix by a constant prefactor $\mathrm{e}^{K_t^\star}$. This modification affects the free energy density (or the Hamiltonian) by a constant only and does not change the thermodynamic properties. In the Hamiltonian limit $K_s \to 0$, $K_t \to \infty$ with fixed $\lambda = K_s/K_t^\star$, we obtain the Hamiltonian of the quantum Potts chain

$$\hat{\mathbf{H}} = -\frac{1}{2}\lambda\sum_{j=1}^{L}\sum_{p=1}^{q-1}(\hat{\mathbf{C}}_j^\dagger\hat{\mathbf{C}}_{j+1})^p - \frac{1}{2}\sum_{j=1}^{L}\sum_{p=1}^{q-1}\hat{\mathbf{R}}_j^p. \tag{64}$$

It is easy to check that in the case $q = 2$, we recover the Hamiltonian (41) of the quantum Ising chain with $\hat{\mathbf{C}}$ playing the role of $\hat{\boldsymbol{\sigma}}_z$ and $\hat{\mathbf{R}}$ that of $\hat{\boldsymbol{\sigma}}_x$. The limit $\lambda \to \infty$ leads to q degenerate ordered ground states $|n, n, n, \ldots, n\rangle$, $n = 0, 1, \ldots, q-1$, while in the other limit $\lambda \to 0$, the term in $\hat{\mathbf{R}}_j$ introduces disorder in the ground state through local rotations between $\hat{\mathbf{C}}_j$-eigenstates. The critical point of the classical two-dimensional model is given by duality, $(\mathrm{e}^{qK_s} - 1)(\mathrm{e}^{qK_t} - 1) = q$, i.e. $K_s = K_t^\star$ or $\lambda_c = 1$.

A different, but simpler route in order to get the time contribution to the Hamiltonian matrix is the following: in the "row states basis" $|\{\nu_j\}\rangle$, the time contribution $\prod_k \mathrm{e}^{K_t(q\delta_{\nu_k,\nu'_k}-1)}$ is a product over "single bond time transfer operators"

$$\texttt{time contribution to}\ \hat{\mathbf{T}} \equiv \prod_k \sum\nolimits_{\{\nu_j\},\{\nu'_j\}} |\{\nu'_j\}\rangle \mathrm{e}^{K_t(q\delta_{\nu_k,\nu'_k}-1)}\langle\{\nu_j\}| \tag{65}$$

which take values $\mathrm{e}^{K_t(q-1)}$ on the diagonal and the same value e^{-K_t} for all single spin flipping terms, e^{-2K_t} for simultaneous double spin flipping terms and so on. Anticipating further simplifications which occur while taking the Hamiltonian limit $K_t \to \infty$, we restrict ourselves to single flipping terms. We introduce the symbol $\sum'_{\{\nu_j\},\{\nu'_j\}}$ with the meaning of a double sum over row states $|\{\nu_j\}\rangle$ and $|\{\nu'_j\}\rangle$ such that $\forall j \neq k$, $\nu'_j = \nu_j$ (single spin flipping terms, since only ν_k is likely to be flipped between the two row states). The contribution to the Hamiltonian follows from taking the logarithm of this expression which leads to $-\epsilon\hat{\mathbf{H}}$.

$$\begin{aligned}\ln(\texttt{time contribution to}\ \hat{\mathbf{T}}) = \sum_k \ln\Big[\mathrm{e}^{K_t(q-1)}\big(\hat{\mathbf{1}} + \\ \mathrm{e}^{-qK_t}\sum\nolimits'_{\substack{\{\nu_j\},\{\nu'_j\}\\ \nu'_k\neq\nu_k}} |\{\nu'_j\}\rangle\langle\{\nu_j\}|\big) + O(\mathrm{e}^{-(q+1)K_t})\Big] \\ \simeq LK_t(q-1) + \mathrm{e}^{-qK_t}\sum\nolimits'_{\substack{\{\nu_j\},\{\nu'_j\}\\ \nu'_k\neq\nu_k}} |\{\nu'_j\}\rangle\langle\{\nu_j\}|\end{aligned} \tag{66}$$

in the limit of a strong coupling in the time direction, $K_t \to \infty$.

4.2. Symmetries

We proceed as in the Ising case to get the symmetries of the Hamiltonian. The classical Potts model is obviously globally unchanged by the cyclic transformation $\forall j$, $0_j \to 1_j$, $1_j \to 2_j$, $\dots (q-1)_j \to 0_j$. Such a rotation in spin states is realized by the operator $\hat{\mathbf{R}}_j$. We may thus define a charge operator which simultaneously rotates Potts variables at all sites,

$$\hat{\mathbf{Q}} = \prod_j \hat{\mathbf{R}}_j. \tag{67}$$

Using the commutation relations between the $\hat{\mathbf{R}}_j$'s and the $\hat{\mathbf{C}}_j$'s, it is easy to prove that the charge operator commutes with the Hamiltonian. Since the eigenvalues of $\hat{\mathbf{R}}_j$ are the q distinct complex numbers $\omega_j = \mathrm{e}^{2i\pi r_j/q}$, those of the charge operator are also given by q numbers $\exp(\sum_j 2i\pi r_j/q)$ which enable to write the Hamiltonian matrix under a block-diagonal structure with q different sectors, depending on the value of $\sum_j r_j \mod(q)$ (the sectors can be referred to as sector # 0, 1, …, $q-1$).

Any operator $\hat{\mathbf{O}}_p$ with the commutation property $\hat{\mathbf{O}}_p\hat{\mathbf{Q}} = \mathrm{e}^{2i\pi p/q}\hat{\mathbf{Q}}\hat{\mathbf{O}}_p$ ($\hat{\mathbf{R}}$ is such an example with $p=0$, $\hat{\mathbf{C}}^\dagger$ is an example with $p=1$, and $\hat{\mathbf{C}}$ with $p=q-1$) has non vanishing matrix elements between states of defined symmetry provided that the charge sectors obey a simple relation $\nu_\psi - \nu_\phi = p$:

$$\begin{aligned}&\forall|\phi\rangle, |\psi\rangle \text{ such that } \hat{\mathbf{Q}}|\phi\rangle = \mathrm{e}^{2i\pi\nu_\phi/q}|\phi\rangle, \hat{\mathbf{Q}}|\psi\rangle = \mathrm{e}^{2i\pi\nu_\psi/q}|\psi\rangle,\\ &\nu_\psi - \nu_\phi \neq p \Rightarrow \langle\phi|\hat{\mathbf{O}}_p|\psi\rangle = 0\end{aligned} \tag{68}$$

As an energy density, we may choose any single term appearing inside the Hamiltonian, e.g. $\texttt{Energy density} = \hat{\mathbf{R}}_j$. A measure of the order parameter would be provided by $\texttt{Local order parameter} = \hat{\mathbf{C}}_j$, or $\hat{\mathbf{C}}_j^\dagger$ as well. The energy density gives access to the critical exponent x_ϵ. For the order parameter, although the two choices correspond to different values of p, since two critical exponents are sufficient in order to determine the whole universality class, the same value of x_σ is expected from both definitions. From gap scaling in particular, we expect $(q-1)$-fold degeneracy of the sectors $p \neq 0$.

4.3. Diagonalization of small chains

In the case of a quantum 3−state Potts chain of length $L = 2$ with periodic boundary conditions, the action of the Hamiltonian in the $\hat{\mathbf{C}}$−operators eigenbasis is the following,

$$\begin{aligned}-2\hat{\mathbf{H}}|\nu_1,\nu_2\rangle &= 2\lambda(\omega_1\omega_2^{-1} + \omega_1^2\omega_2^{-2})|\nu_1,\nu_2\rangle\\ &\quad + |\nu_1+1,\nu_2\rangle + |\nu_1+2,\nu_2\rangle + |\nu_1,\nu_2+1\rangle + |\nu_1,\nu_2+2\rangle, \quad (69)\\ \omega_j &= \exp(2i\pi\nu_j/3). \quad (70)\end{aligned}$$

We obtain the following $3^2 \times 3^2$ matrix,

$$[-2\hat{\mathbf{H}}] = \begin{pmatrix} 4\lambda & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & -2\lambda & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & -2\lambda & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -2\lambda & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 4\lambda & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & -2\lambda & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & -2\lambda & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & -2\lambda & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 4\lambda \end{pmatrix} \begin{matrix} |00\rangle_C \\ |01\rangle_C \\ |02\rangle_C \\ |10\rangle_C \\ |11\rangle_C \\ |12\rangle_C \\ |20\rangle_C \\ |21\rangle_C \\ |22\rangle_C \end{matrix} \tag{71}$$

the eigenvalues of which are (eigenvalues of $\hat{\mathbf{H}}$ at $\lambda_c = 1$), -2.732, -2.137, -2.137, $+0.500$, $+0.500$, $+0.732$, $+1.637$, $+1.637$, and $+2.000$. It is of course more efficient to exploit the symmetries and to work in the $\hat{\mathbf{R}}-$operators eigenbasis where,

$$\begin{aligned} -2\hat{\mathbf{H}}|r_1, r_2\rangle &= 2\lambda(|r_1+1, r_2-1\rangle + |r_1+2, r_2-2\rangle) \\ &\quad + (\omega_1 + \omega_1^2 + \omega_2 + \omega_2^2)|r_1, r_2\rangle, \end{aligned} \tag{72}$$

$$\omega_j = \exp(2i\pi r_j/3). \tag{73}$$

The corresponding matrix is now

$$[-2\hat{\mathbf{H}}] = \begin{pmatrix} 4 & 2\lambda & 2\lambda & & & & & & \\ 2\lambda & -2 & 2\lambda & & & & & & \\ 2\lambda & 2\lambda & -2 & & & & & & \\ & & & -2 & 2\lambda & 2\lambda & & & \\ & & & 2\lambda & 1 & 2\lambda & & & \\ & & & 2\lambda & 2\lambda & 1 & & & \\ & & & & & & -2 & 2\lambda & 2\lambda \\ & & & & & & 2\lambda & 1 & 2\lambda \\ & & & & & & 2\lambda & 2\lambda & 1 \end{pmatrix} \begin{matrix} |00\rangle_R \\ |12\rangle_R \\ |21\rangle_R \\ |11\rangle_R \\ |20\rangle_R \\ |02\rangle_R \\ |22\rangle_R \\ |01\rangle_R \\ |10\rangle_R \end{matrix} \tag{74}$$

It is block diagonal, with eigenvalues of the first block (0 sector) -2.732, $+0.732$ and $+2.000$, and the two-fold degenerate eigenvalues of the two remaining identical blocks (sectors 1 and 2), -2.137, $+0.500$ and $+1.637$. The ground state and energy eigenstates are given by $|\texttt{Gnd}\rangle = a^{00}_{\texttt{Gnd}}|00\rangle + a^{12}_{\texttt{Gnd}}|12\rangle + a^{21}_{\texttt{Gnd}}|21\rangle$ and $|\texttt{Energy}\rangle = a^{00}_{\texttt{Energy}}|00\rangle + a^{12}_{\texttt{Energy}}|12\rangle + a^{21}_{\texttt{Energy}}|21\rangle$ and the energy density follows

$$\begin{aligned} \langle \texttt{Energy density}\rangle &= |\langle \texttt{Energy}|\hat{\mathbf{R}}_1|\texttt{Gnd}\rangle| \\ &= |a^{00}_{\texttt{Energy}}a^{00}_{\texttt{Gnd}} + a^{12}_{\texttt{Energy}}a^{12}_{\texttt{Gnd}}\mathrm{e}^{2i\pi/3} + a^{21}_{\texttt{Energy}}a^{21}_{\texttt{Gnd}}\mathrm{e}^{4i\pi/3}| \\ &= 0.613. \end{aligned} \tag{75}$$

In the $p = 1$ sector, the order parameter density is given by (the notation is obvious)

$$\begin{aligned} \langle \texttt{Order parameter}\rangle &= |\langle \texttt{Order } p=1|\hat{\mathbf{C}}_1^\dagger|\texttt{Gnd}\rangle| \\ &= |a^{10}_{\texttt{Order}}a^{00}_{\texttt{Gnd}} + a^{22}_{\texttt{Order}}a^{12}_{\texttt{Gnd}} + a^{01}_{\texttt{Order}}a^{21}_{\texttt{Gnd}}| \\ &= 0.916, \end{aligned} \tag{76}$$

and, due to the complete degeneracy of the two sectors $p = 1$ and $p = 2$, we get the same result in the remaining sector

$$\begin{aligned} \langle \texttt{Order parameter}\rangle &= |\langle \texttt{Order } p=2|\hat{\mathbf{C}}_1|\texttt{Gnd}\rangle| \\ &= |a^{20}_{\texttt{Order}}a^{00}_{\texttt{Gnd}} + a^{02}_{\texttt{Order}}a^{12}_{\texttt{Gnd}} + a^{11}_{\texttt{Order}}a^{21}_{\texttt{Gnd}}| \\ &= 0.916, \end{aligned} \tag{77}$$

Table 3. Values of the physical properties of small quantum 3− (upper part of the table) and 4−state (lower part of the table) Potts chains.

L	$E_{\texttt{Gnd}}$	$E_{\texttt{Energy}}$	$E_{\texttt{Order}}$	$\langle\texttt{Energy density}\rangle$	$\langle\texttt{Order parameter}\rangle$
2	−2.732	0.732	−2.137	0.613	0.916
3	−3.842	−1.500	−3.462	0.505	0.867
2	−4.000	0.000	−3.236	0.577	0.909
3	−5.606	−3.000	−5.123	0.480	0.858

The relevant eigenvalues and matrix elements for systems of sizes $L = 2$ and 3 are collected in table 3.

Interested readers might find helpful to have also the matrix representing the 4−state Potts chain. When $L = 2$ (the matrix is now $4^L \times 4^L$) at the critical coupling $\lambda_c = 1$ in its block diagonal form in the $\hat{\mathbf{R}}$−eigenbasis $\{|00\rangle, |13\rangle, |22\rangle, |31\rangle, |01\rangle, |10\rangle, |23\rangle, |32\rangle, |02\rangle, |11\rangle, |20\rangle, |33\rangle, |03\rangle, |12\rangle, |21\rangle, |30\rangle\}$, this matrix reads as

$$[-2\hat{\mathsf{H}}] = \begin{pmatrix} \begin{vmatrix} 6 & 2 & 2 & 2 \\ 2 & -2 & 2 & 2 \\ 2 & 2 & -2 & 2 \\ 2 & 2 & 2 & -2 \end{vmatrix} & & & \\ & \begin{vmatrix} 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 \\ 2 & 2 & -2 & 2 \\ 2 & 2 & 2 & -2 \end{vmatrix} & & \\ & & \begin{vmatrix} 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 \\ 2 & 2 & -2 & 2 \\ 2 & 2 & 2 & -2 \end{vmatrix} & \\ & & & \begin{vmatrix} 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 \\ 2 & 2 & -2 & 2 \\ 2 & 2 & 2 & -2 \end{vmatrix} \end{pmatrix} \tag{78}$$

The following section, where an approximate determination of the critical exponents of the 3− and 4−state Potts models will be proposed, will make use of the numerical values listed in table 3.

5. Discussion

Finite-size estimators of the critical exponents follow from equations (18) and (19),

$$x_\phi = \frac{\ln \phi(L) - \ln \phi(L')}{\ln L - \ln L'}. \tag{79}$$

The results, collected in table 4 in the case of the Ising, 3− and 4−state Potts models, show as expected a very weak convergence. A strip of width 2 to 4 is obviously a poor approximation of the thermodynamic limit. In the case of the Ising model, exact diagonalization [8, 12] through Jordan-Wigner transformation into fermion operators, then Bogoljubov-Valatin canonical transformation into free fermions leads to an exact expression for the energy density [13]

$$\langle\texttt{Energy density}\rangle = \frac{2}{L}\cos\left(\frac{\pi}{2L}\right). \tag{80}$$

Unfortunately, there is no closed expression for the order parameter matrix element which couples two different sectors of the Hamiltonian. Hence, the presence of a boundary term breaks the quadratic expression necessary for the diagonalization.

Table 4. Estimators of critical exponents from FSS of local properties of small quantum Ising and 3− and 4−state Potts chains.

Ising				3−state Potts				4−state Potts			
L	L'	x_ϵ	x_σ	L	L'	x_ϵ	x_σ	L	L'	x_ϵ	x_σ
2	3	0.501	0.120	2	3	0.478	0.136	2	3	0.454	0.142
3	4	0.773	0.129	–	–	–	–	–	–	–	–
∞		1.000	0.125	∞		0.800	0.133	∞		0.500	0.125

The resort to gap scaling (23) as predicted from conformal invariance is thus desirable. Indeed, as emphasized in Section 2, the cylinder geometry is the geometrical shape of the classical problem corresponding to the one-dimensional quantum chain. Since such an infinitely long cylinder follows from the infinite plane geometry through conformal mapping, we may argue that the thermodynamic limit is somehow encoded in the results following from conformal rescaling and a better convergence for the critical exponents is expected. With the normalization of equation (41) the fermion excitations take the form $\varepsilon_k = |2\sin\frac{k}{2}|$. The sound velocity is thus fixed to unity as previously announced. The results following from gap scaling,

$$x_\phi = \frac{L \times \mathtt{gap}_\phi}{2\pi v_s}, \tag{81}$$

are collected in table 5. The quality of the results is indisputably better than through FSS.

In the case of the Potts model, the sound velocity is not known and it is worth referring to the literature. Gehlen et al. have studied numerically quantum Potts chains in refs. [7, 14] where tables of numerical results are reported for $q = 3$ up to a size $L = 13$ and for $q = 4$ up to $L = 11$ (they denote R (P) the energy gap (magnetic gap) multiplied by the strip size) . These authors used a different normalization and their Hamiltonian for $q = 3$ in [14] is related to ours through $\frac{2}{3}\hat{\mathbf{H}}_{\mathtt{here}}(q=3) + \frac{4}{3}\hat{\mathbf{1}} = \hat{\mathbf{H}}_{\mathtt{Gehlen}}(q=3)$, while in [7] it is related to ours through $\hat{\mathbf{H}}_{\mathtt{here}}(q=4) = 2\hat{\mathbf{H}}_{\mathtt{Gehlen}}(q=4)$. Using the values of the sound velocity quoted in [7], we deduce that in our case the sound velocity is 3/2 larger for $q = 3$ and 2 times larger for $q = 4$, i.e.

$$v_s(q=3) = 1.299, \quad v_s(q=4) = 1.578. \tag{82}$$

These values are used to calculate the exponents reported in table 5. Further numerical values denoted with an asterisk are taken from refs. [7, 14] to complete the table with results at larger sizes. The expected result in the thermodynamic is also mentioned in the table [15].

To summarize, we note that the quality of the results is acceptable for the relatively small effort of diagonalization of small matrices. The quest for critical exponents is an important step in the characterization of the nature of a phase transition, since these quantities are universal. The study of models of statistical physics which display second-order phase transitions usually requires sophisticated methods, and approximate determinations are often desirable. Considering quite small systems, we reach a few percent accuracy in the determination of the critical exponents in the case of the Ising and 3−state Potts models. The convergence is poor in the

Table 5. Estimators of critical exponents from gap scaling of small quantum Ising, 3−state and 4−state Potts chains. An asterisk indicates that the numerical value was extracted from refs. [7, 14] according to the transformation mentioned above, $x = 3R/4\pi v_s$ for $q = 3$ and $x = R/\pi v_s$ for $q = 4$.

Ising			3−state Potts			4−state Potts		
L	x_ϵ	x_σ	L	x_ϵ	x_σ	L	x_ϵ	x_σ
2	0.900	0.132	2	0.848	0.145	2	0.807	0.154
3	0.955	0.128	3	0.861	0.139	3	0.788	0.146
4	0.975	0.127	4	0.857	0.137	4	$0.767^\star$	$0.143^\star$
			13	$0.848^\star$	$0.134^\star$	11	$0.700^\star$	$0.137^\star$
∞	1.000	0.125	∞	0.800	0.133	∞	0.500	0.125

4−state Potts case. This is essentially due to the logarithmic corrections present in this model.

Eventually, regarding the relatively small efforts, we believe that an introduction to the study of quantum chains in courses on statistical physics or many-body problems might be of interest.

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