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# Numerical tests of local scale invariance in ageing q-state Potts models

E. Lorenz and W. Janke

*Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig Augustusplatz 10/11, 04109 Leipzig, Germany*

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**Abstract** – Much effort has been spent over the last years to achieve a coherent theoretical description of ageing as a non-linear dynamics process. Long supposed to be a consequence of the slow dynamics of glassy systems only, ageing phenomena could also be identified in the phase-ordering kinetics of simple ferromagnets. As a phenomenological approach Henkel *et al.* developed a group of *local* scale transformations under which two-time autocorrelation and response functions should transform covariantly. This work is to extend previous numerical tests of the predicted scaling functions for the Ising model by Monte Carlo simulations of two-dimensional $q$-state Potts models with $q=3$ and 8, which, in equilibrium, undergo temperature-driven phase transitions of second and first order, respectively.



**Introduction.** – Phase ordering as a non-equilibrium process following a temperature quench from a completely disordered state at $T_1=\infty$ to a temperature $T_2\leqslant T_c$ in the ordered phase of systems with a non-conserved order parameter is a well-known phenomenon [1], but it has recently attracted new attention through studies of ageing phenomena. Ageing could be observed in a broad variety of systems with slow relaxation dynamics. But rather than considering genuine glassy systems, better insights can be gained through the consideration of phase-ordering kinetics in physically simpler ferromagnets.

In this work we investigated isotropic $q$-state Potts models with Hamiltonian [2]

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}-\bar{h}\sum_i\delta_{\sigma_i,h_i}\quad\text{with } \sigma_i=1,\ldots,q, \qquad (1)$$

where $\delta_{\cdot,\cdot}$ is the Kronecker symbol and $h_i$ is a $q$-valent auxiliary field with amplitude $\bar{h}$. For $\bar{h}=0$, the critical temperature is exactly known to be $k_BT_c/J=1/\ln(1+\sqrt{q})$ [3,4]. In two dimensions, the phase transition is continuous (second order) for $q\leqslant 4$ and of first order for $q>4$, respectively, for all lattice types [2–4]. As typical representatives, we studied the cases $q=2,3$ and 8.

Starting from a fully disordered state, a quench into the ferromagnetic phase at time $t=0$ is followed by the formation of long-range correlations or, in a more descriptive language, by the formation and growth of local regions of parallel spins called domains or clusters. A single spin loses its ability to orientate non-parallel to its neighbours with decreasing temperature, according to the fact that the entropy contribution to the free energy for $T<T_c$ becomes weaker than the spin-spin coupling. Inside a domain a spin is quite stable in comparison to a spin at its surface. The dynamics of the system is therefore mainly governed by the movement of domain walls. In order to minimize the energy expensive domain surfaces in the system, domains grow and straighten their surface. The typical correlated length scale grows with time $t$ as $L\sim t^{1/z}$, where $z$ is the dynamical exponent which, in the case of simple ferromagnets with a scalar order parameter and a quench to $T_2<T_c$, is known to be $z=2$, using simple diffusion or random-walk arguments [5]. For a quench to the critical temperature $T_2=T_c$ itself, where fluctuations on all length scales become important, this exponent takes a somewhat larger value, *e.g.*, for the two-dimensional Ising model one finds $z\approx 2.17$ [6].

**Ageing phenomena and scale invariance.** – The relaxation process after a quench happens on a growing time scale. This can be revealed by measurements of two-time quantities $f(t,s)$ which no longer transform time-translation invariantly as they would do for small perturbations in equilibrium, *i.e.*, they are not only a function of the time difference $t-s>0$. Instead, in phase-ordering kinetics they depend non-trivially on the ratio of the two times $t/s$, where $s$ is the so-called waiting time and $t>s$ the observation time. The dependence of the relaxation on the waiting time $s$ is the notional origin of ageing: older samples respond more slowly.

Commonly considered quantities exhibiting ageing phenomena are the two-time autocorrelator and the two-time response function

$$C(t,s)=\langle\phi(t)\phi(s)\rangle\,,\qquad R(t,s)=\left.\frac{\partial\langle\phi(t)\rangle}{\partial h(s)}\right|_{h(s)=0},\quad (2)$$

where the local order parameter $\phi$ stands generically for a local field or spin. Being far from equilibrium, ageing systems are not time-translation invariant and hence break the fluctuation-dissipation theorem (FDT) as quantified by the deviation of $X(t,s)=TR(t,s)/\partial_s C(t,s)$ from unity [7]. It could be shown that $X$ is not a function of $C(t,s)$ only, but depends nontrivially on $t/s$ [8,9]. In the case of critical relaxation with $T_2=T_c$, the asymptotic value $X_\infty=\lim_{s\to\infty}(\lim_{t\to\infty}X(t,s))$ was found to be universal, depending on a universal amplitude ratio and critical exponents [6].

In the ageing regime, where $s$ and $t-s$ are much larger than the microscopic time scale, dynamical scaling predicts for the autocorrelator and the response function of a broad variety of models the scaling laws [10,11]

$$C(t,s)\sim s^{-b}f_C(t/s)\,,\qquad R(t,s)\sim s^{-1-a}f_R(t/s)\,.\quad (3)$$

In the asymptotic limit $x\equiv t/s\gg 1$, the scaling functions fall off as

$$f_C(x)\sim x^{-\lambda_C/z}\,,\qquad f_R(x)\sim x^{-\lambda_R/z}\,,\quad (4)$$

with clear evidence for $\lambda_C=\lambda_R$ in the case of quenches below $T_c$ with short-range initial correlations (and a Galilei invariant "noiseless" $T=0$ limit) [12]. For the Ising model in $d=2$ dimensions and non-zero temperatures $T_2<T_c$, the numerical estimate $\lambda\approx 1.25$ was found to saturate the bound $\lambda\leqslant 5/4$ [13]. For $T_2<T_c$, one furthermore has $b=0$ because $C(t,s)$ falls off from $C(t=s,s)=1$, but there is no general result for $a$. In the Ising model with Glauber dynamics, $a=1/z=1/2$ is conjectured for $d=2,3$ dimensions [14] (see also the discussion below) while for the spherical model $a=d/2-1$ for $d>2$ [15], assuming a fully disordered initial state. For a critical quench to $T_2=T_c$, the dynamical exponents $a$ and $b$ can be related to static critical exponents as $a=b=2\beta/(\nu z)$ [6,15] and $\lambda_C=\lambda_R=d+x-x_i$, where $x=\beta/\nu$ and $x_i$ denote the scaling dimension of the order parameter and the initial magnetization, respectively [6].

**Local scale invariance.** – The dynamics of ageing systems may be thought of as being described by a Langevin equation (LE) [12,16,17]. In the growth law $L\sim t^{1/z}$, the dynamical exponent $z$ acts as an anisotropy exponent ($\theta$) between spatial and temporal dimensions. Henkel *et al.* [16,17] proposed a possible approach in which the dynamical scale invariance $t\to b^z t$, $\mathbf{r}\to b\mathbf{r}$ is extended to *local* scale invariance (LSI) with a position-dependent dilatation factor $b(\mathbf{r})$. Known special cases of LSI are conformal invariance for $\theta=1$ and Schrödinger invariance for $\theta=2$. The exclusion of time translations then leads to a certain subalgebra $\mathcal{S}$ [17], whose generators $X$ give rise to a set of differential equations with application of the covariance condition $XR(t,s)=0$. This can be solved and after a comparison with the expected scaling form (3), the response scaling function can be written as [16,17]

$$f_R(x)=r_0x^{1+a+\lambda_R/z}(x-1)^{-1-a}.\quad (5)$$

Hence, if $a$ and $\lambda_R/z$ are known, the whole functional form is determined up to a normalization constant $r_0$. The spatio-temporal form of the response function in (2) (with $\phi(t)\to\phi(t,\mathbf{x})$, $h(s)\to h(s,\mathbf{x}')$ and $\mathbf{r}=\mathbf{x}-\mathbf{x}'$) is given with explicit use of Galilei invariance as [17] $R(t,s;\mathbf{r})=R(t,s)\exp(-(\mathcal{M}/2)[r^2/(t-s)])$, where $\mathcal{M}\equiv 1/2D$ is a non-universal mass parameter of the field $\phi$.

The autocorrelator $C(t,s)$ can be obtained by integrating over noiseless spatio-temporal three-point response functions which can be derived through a gauge transformation, mapping the LE to the free Schrödinger equation [12]. Making use of the well-known three-point response functions for a Schrödinger invariant theory [18], an explicit form of $C(t,s)$ could be derived which, after a comparison with the scaling relation (3), can be written as [12]

$$C(x=t/s)=x^{\lambda_C/z}(x-1)^{-2\lambda_C/z}\Phi\left(\frac{x+1}{x-1}\right).\quad (6)$$

To obtain the scaling function $\Phi(w)$, the Schrödinger group has to be extended by considering $\mathcal{M}$ as a dynamical variable [19,20]. The dynamical symmetry group then extends to the conformal group in $d+2$ dimensions and two additional generators can be identified [21]. Those, together with the conservation of the masses of the fields [18], were then used to obtain a fairly lengthy explicit expression for $\Phi(w)$ involving hypergeometric and incomplete Gamma functions together with three non-universal constants $A$, $B$ and $E$, which is given in eqs. (11) and (17) of ref. [19] and shall not be reproduced here.

**Numerical tests.** – To test the scaling predictions derived from LSI, we performed extensive Monte Carlo simulations of two-dimensional 2-, 3- and 8-states Potts models with non-conserved order parameter on a square lattice of size $N=L^2$ with periodic boundary conditions. For Glauber dynamics we evolved the systems with the heatbath algorithm. Instead of randomly selecting the spins to be updated as done in refs. [16,19,22,23],

Table I: The quench temperature and all determined free parameters of the scaling functions. For a comparison to the $q=2$ measurements in ref. [19] we assumed the values for $A$, $B$ and $E$ given there.

| | $T_2$ | $\lambda_C$ | $A$ | $B$ | $E$ | $r_0$ | $r_1$ |
|---|---|---|---|---|---|---|---|
| $q=2$ | 0.7500 | 1.24(2) | −5.41 | 18.4 | 1.24 | 1.24(2) | −1.18(2) |
| $q=3$ | 0.4975 | 1.19(3) | −0.05 | 2.15 | 0.6 | 1.01(1) | −0.91(1) |
| $q=8$ | 0.3725 | 1.25(1) | −0.07 | 1.98 | 0.4 | 0.55(1) | −0.50(2) |

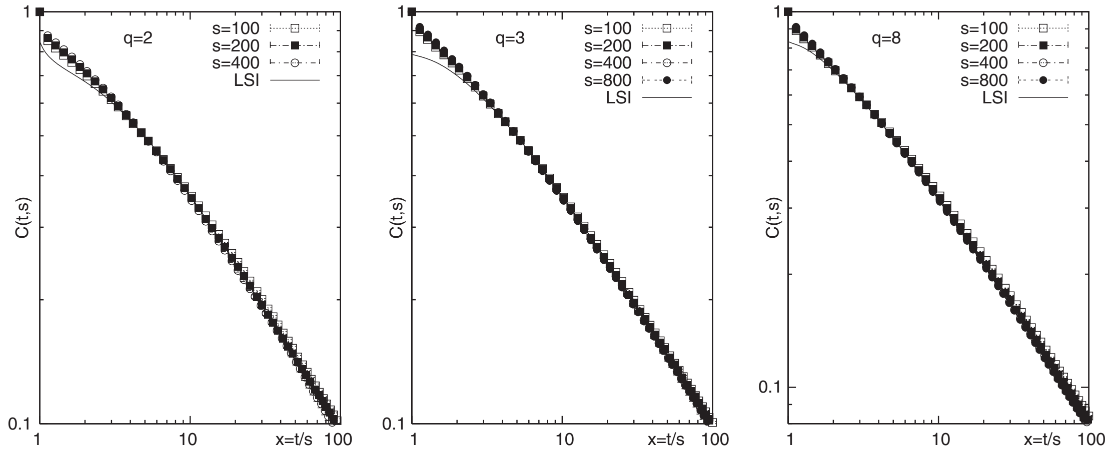


Fig. 1: Scaling behaviour of the autocorrelator for two-dimensional $q$-state Potts models with $q=2,3$ and 8 in comparison with the prediction from LSI. The error bars are smaller than the data symbols.

we implemented the checkerboard update scheme because of run-time advantages. This affects only the non-universal amplitudes of the response function by a uniform factor. To prepare the initial state at $T_1=T_\infty$, we let the spins take one of the possible $q$ states with the same probability, taking special care that $M(t=0)\approx 0$ to prevent the initial rising of the magnetization known from short-time dynamics. After preparation, the $q=3,8$ systems were quenched to $T_2\approx T_c/2$ (cf. table I). This is a good compromise to prevent a crossover to critical behaviour on the one hand and to verify scaling with $z=2$ for non-zero temperatures $T_2>0$ on the other. The $q=2$ model was quenched to $T_2=0.75\approx 0.66\,T_c$ in order to enable a comparison with previous numerical tests made with the random update scheme.

*Autocorrelation.* To test the scaling function for the autocorrelator (eqs. (11) and (17) in ref. [19]) we measured the autocorrelation function of the Potts models according to

$$C(t,s)=\langle\phi(t)\phi(s)\rangle=\frac{1}{q-1}\left(\frac{q}{N}\sum_{i=1}^{N}\left\langle\delta_{\sigma_i(t),\sigma_i(s)}\right\rangle-1\right), \tag{7}$$

where the sum yields the lattice average and the angular brackets mean an average over several runs with different initial states and thermal noise. To prevent early finite-size effects for simulation times up to $s=800$ and $x=100$ (*i.e.*, $t=80000$), we had to use a lattice of size $L=1600$. The usage of the checkerboard update scheme accelerates the domain-growth with a factor larger than 2 in comparison to the random update scheme which can be explained straightforwardly by the fact that in a random update only about $N/e$ different spins are touched on the average within a sweep[1]. The advantage in computer time compensates the additional expenses of larger systems easily (at least in our implementations). The measurements for the $q=2$ model were done for $L=800$ only up to $s=400$. This was sufficient to ensure the equivalence with the data presented in ref. [19]. For the models with $q=3$ and 8, measurements up to $s=200$ were carried out for $L=800$, and for $s=400,800$ on the larger $L=1600$ systems. For averages and error bars, 500 runs with different random initial states were recorded for $L=800$ and 125 runs on the $L=1600$ systems. Our data shown in fig. 1 clearly confirm the expected dynamical scaling behaviour (3).

To proceed with the test of *local* scale invariance, we first estimated the exponent $\lambda_C$ from a fit of $C(t,s)\simeq C_\infty x^{-\lambda_C/z}$ in the interval $x\in[80,100]$ for the largest waiting times $s$. In all three cases, our results given

[1]Note that consequently also the waiting time $s$ is not directly comparable to that in random updates.

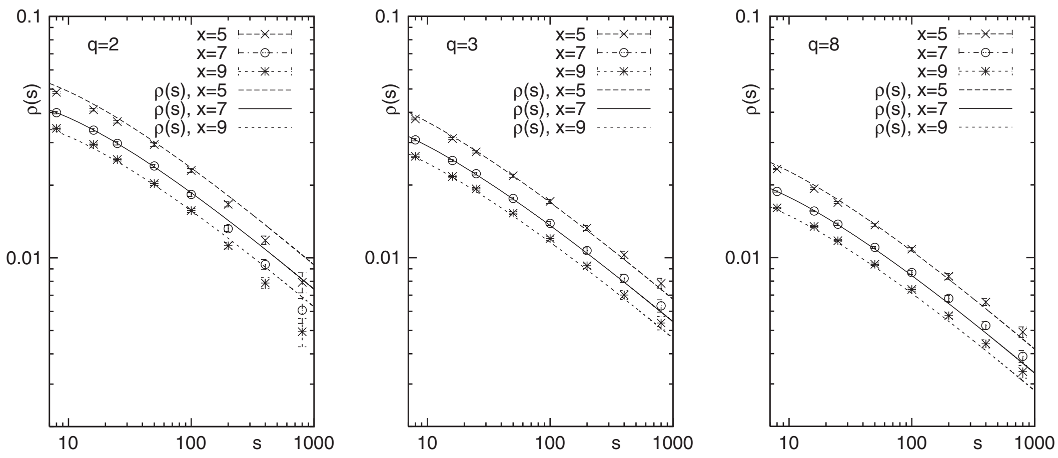


Fig. 2: Scaling of $\rho(t,s) = TM_{\text{TRM}}/\bar{h}$ as a function of the waiting time $s$ for several fixed $x = t/s$. The middle solid curve shows $\hat{\rho}(s) \equiv \rho(xs, s)$ fitted in $r_0$ and $r_1$ to the data for $x = 7$. The other two dashed lines correspond to the resulting predictions for $x = 5, 9$.

in table I are compatible with $\lambda_C = 5/4$. The apparent constancy, however, should be taken with care since only a relatively small range of $q$ values is covered. In fact, in a $T = 0$ study [24] a variation of $\lambda_C$ from around 1.25 for $q = 2$ to 2 for $q = \infty$ was observed. Next the three non-universal parameters $A$, $B$ and $E$ of the autocorrelation scaling function in eqs. (11) and (17) of ref. [19] were obtained through a 3-parameter fit by taking into account two additional constraints as described in ref. [19]. Both the amplitude $C_\infty$ in $C(t,s) \simeq C_\infty x^{-\lambda_C/z}$ and the crossing point of the data for different $s$ were used. Nevertheless the 3-parameter fit stays a challenge for standard fit routines (Levenberg-Marquard, etc.), so we were not able to give firm error estimations. With the parameters $A$, $B$ and $E$ given in table I in reliable precision, we find in fig. 1 in all three cases good agreement of the LSI prediction with our data for $x = t/s \gtrsim 2$–3.

*Response.* Because of heavy fluctuations in direct measurements of the response function, one commonly considers an integrated response, either the zero-field–cooled susceptibility $\chi_{\text{ZFC}} = T\int_s^t \mathrm{d}u R(t,u)$ or the thermo-remanent magnetization $M_{\text{TRM}}$,

$$\rho(t,s) = \frac{T}{\bar{h}(s)} M_{\text{TRM}} = \int_0^s \mathrm{d}u\, R(t,u) = \frac{T}{\bar{h}(s)} \frac{1}{q-1} \left( \frac{q}{N} \sum_{i=1}^{N} \overline{\langle \delta_{\sigma_i(t), h_i(s)} \rangle} - 1 \right), \quad (8)$$

where the measurement protocol is as follows. During the waiting time $[0, s]$ a spatially random magnetic field is turned on in the Hamiltonian (1), where the $h_i$ are chosen to take on one of the $q$ values $1, \ldots, q$ randomly to prevent that one of the $q$ phases will be favoured, and its amplitude was set to a small value $\bar{h} = 0.05$ to keep the response linear. During the waiting time the field is kept fixed and then switched off at time $s$ (*i.e.*, $\bar{h} \propto \Theta(s - t)$ in eq. (1)). The values of the spatially random, but temporally constant magnetic field ($h_i(s)$, $\bar{h}(s)$) are then used in the measurements of (8) also at later times $t > s$. Again the sum over all lattice sites exploits spatial translation invariance, the angular brackets give the mean over different runs and the bar is due to the averaging over different realizations of the magnetic field. The initial configuration, the thermal noise and the random field were varied for every run. With those settings it was possible to measure the response in a system sized $L = 800$ with time ratios up to $x = t/s = 10$ and waiting times up to $s = 800$. The average and standard deviation have then been calculated over 10000 sample runs for each waiting time.

From eq. (5) there follows, for the scaling behaviour of $M_{\text{TRM}}$ [22,23],

$$\rho(t,s) = r_0 s^{-a} f_M(t/s) + r_1 s^{-\lambda_R/z} g_M(t/s), \quad (9)$$

with the explicit scaling function (${}_2F_1$ is the hypergeometric function)

$$f_M(x) = x^{-\lambda_R/z}\, {}_2F_1(1 + a, \lambda_R/z - a;\ \lambda_R/z - a + 1; 1/x) \quad (10)$$

and the crossover correction $g_M(x) \approx x^{-\lambda_R/z}$ also given in ref. [22]. To test the scaling of $M_{\text{TRM}}$, the correction term $s^{-\lambda_R/z} g_M(t/s)$ in (9) has to be subtracted off. This can only be done with knowledge of the exponents $a$, $\lambda_R/z$ and the prefactors $r_0$, $r_1$. Since non-linear 4-parameter fits (of $\rho(t,s)$ as a function of $s$ at fixed $x = t/s$) are notoriously unstable, we proceeded as follows [25]. By systematically scanning values for $a \in [0,1]$ and $\lambda_R \in [1.0, 1.5]$, the problem is effectively reduced to a linear 2-parameter fit in $r_0$ and $r_1$. The landscape of the goodness-of-fit or $\chi^2$ values over the $a$-$\lambda_R$ plane is then a reliable measure for the optimal parameter choice. Whereas the parameter $a$ was found to be rather sharply determined

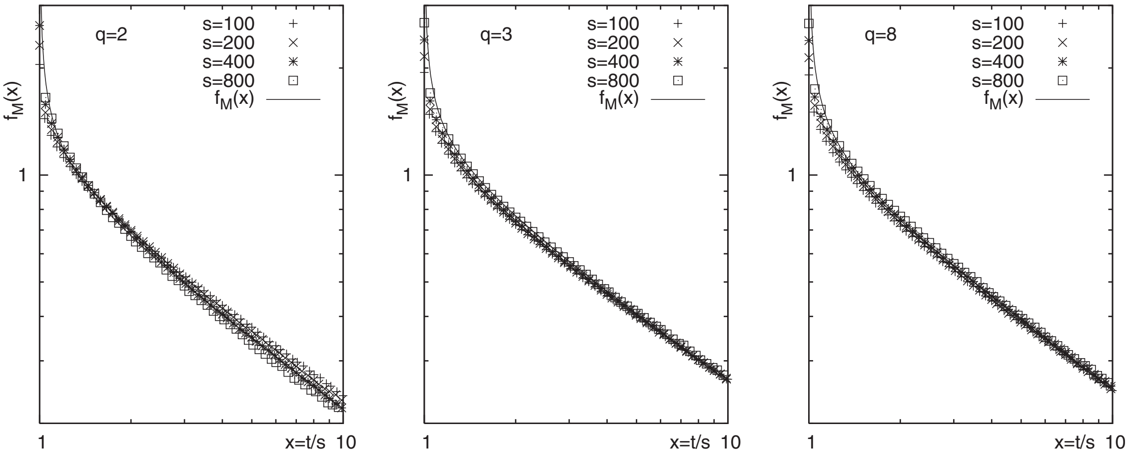


Fig. 3: Scaling of the integrated response scaling function $f_M(x)$ for different waiting times $s$. The full lines correspond to $f_M(x)$ as given in eq. (10) with $a=1/z=1/2$ and $\lambda_R=\lambda_C$ from table I.

($\approx 0.65$, 0.49, 0.51 for $q=2$, 3, 8), the $\chi^2$ landscape exhibits a very shallow valley in the direction of $\lambda_R$, which is thus difficult to determine [26]. We hence assumed that $\lambda_R=\lambda_C$ [12] and took its value from our measurements of $\lambda_C$ in table I. Furthermore, since our estimates are compatible with $a\approx 0.5$ (for $q=2$, see also ref. [22]), we employed the conjecture $a=1/z=1/2$ [14] to obtain the values for $r_0$ and $r_1$ compiled in table I from fits to the $x=7$ data. Plots of $\hat{\rho}(s)\equiv\rho(xs,s)$ for $x=5$, 7 and 9 are shown in fig. 2. With our data and method of analysis, we can thus definitely rule out alternative predictions such as $a=1/4$ [27]. As a possible reason for this discrepancy one may speculate that in ref. [27] much shorter times $s$ and $t-s$ are considered where LSI is not expected to hold.

After subtracting off the correction term in (9) we tested our numerical data against the scaling function $f_M(x)$. As is demonstrated in fig. 3, apart from some deviations in the non-ageing regime where $s,t$ and $x=t/s$ are small, a good agreement of the data with the scaling function derived from LSI can be observed. Note that in comparison to the values given in ref. [23] for the two-dimensional Ising model, our estimates of $r_0$ and $r_1$ using a checkerboard update are less than half in magnitude. Universality of the dynamics is still given. Additional measurements of the spatio-temporal response function confirm the underlying Galilei invariance assumptions. This and further results for other spatially resolved quantities will be reported in a separate publication [25].

**Conclusions.** – We performed extensive Monte Carlo simulations of phase ordering in two-dimensional 2-, 3- and 8-state Potts models on a square lattice and measured the autocorrelation and response function to provide additional numerical tests of local scale invariance as an extension of the known dynamical scaling to a kind of conformal invariance in phase-ordering kinetics. Down to very small values of the scaling variable $x=t/s$ we found good agreement with the scaling functions derived from LSI and thereby support this phenomenological approach to ageing. In particular also the 8-state Potts model, undergoing a temperature-driven first-order phase transition in equilibrium, was found to fit perfectly into this scheme.

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