J. Phys.: Condens. Matter 1 (1989) 8147–8154. Printed in the UK

Critical and finite-size-scaling behaviours of short-range order parameters

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Received 23 February 1989, in final form 22 May 1989

Abstract. We investigate the behaviour of short-range order (SRO) parameters with temperature and system size in several versions of the Ising model, namely the pure and dilute models, the impure case where a fraction of spins are maintained fixed at one of the two possible states, and a driven-diffusive (non-equilibrium) lattice gas. The behaviour shown by SRO parameters is interesting, and reveals itself to be most useful in practice for determining qualitative and quantitative properties of phase transitions.

1. Introduction

The modern theory of phase transitions and critical phenomena has revealed, in particular, that a systematic study of finite-size effects (Ferdinand and Fisher 1969, Fisher 1971, Binder 1972) may uncover the relevant, limiting behaviour characterising a large variety of macroscopic (thermodynamic-limit) systems under very different conditions (see, for instance, Landau 1976, Marro and Toral 1983, Toral and Marro 1985, Labarta *et al* 1986, Challa *et al* 1986, Toral and Wall 1987, Vallés and Marro 1987, Gonzalez-Miranda *et al* 1987, Garrido *et al* 1989). One usually proceeds either from first principles or from empirical scaling expressions (Barmatz *et al* 1975) for some physical quantity as a function of the system size N and of the temperature parameter $\varepsilon \equiv 1 - T/T_c$, where T_c represents the critical temperature of the infinite system, and performs either exact or numerical (e.g. Monte Carlo) computations on finite systems. An outstanding fact is that, while those expressions are defined formally valid in the limit $N \rightarrow \infty$, $\varepsilon \rightarrow 0$, they turn out also to be applicable in practice not so close to T_c and to rather small systems, say to temperatures and sizes which are well within present computational capabilities. As a consequence, finite-size scaling analysis is nowadays an excellent complement to other, more conventional methods such as series expansions and renormalisation group techniques, and they often lead to the best available accuracy (see, for instance, Barber 1983).

A series of recent Monte Carlo analyses, concerning both equilibrium (Labarta *et al* 1986) and non-equilibrium problems (Vallés and Marro 1987, González-Miranda *et al*

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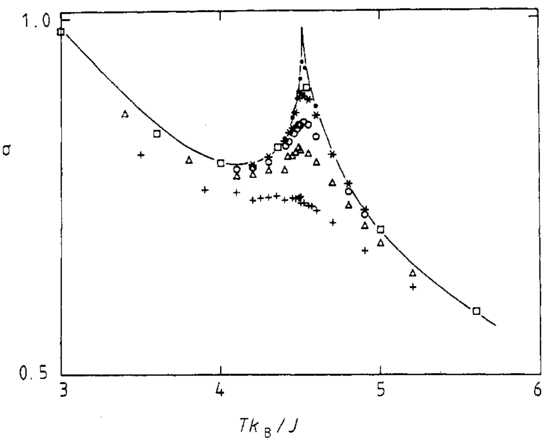

Figure 1. The parameter σ defined in equation (2.1), as a function of temperature, in the case of the pure 3D Ising model as obtained from Monte Carlo computations for sizes $L = 8$ (crosses), 12 (triangles), 16 (open circles), 24 (asterisks), 30 (squares) and 40 (full circles). The full curve represents the value for the infinite system which follows from equation (2.4) by using series expansions for m and u.

1987, Garrido *et al* 1989), revealed to us that the study of short-range order (SRO) may easily allow to clarify most important properties of the phase transition involved. As a matter of fact, SRO parameters behave differently in qualitative terms for every type of phase transition, thus clearly uncovering the nature of the latter. In addition, SRO parameters usually remain bounded at finite temperatures, thus helping to locate the transition temperature and even to compute the critical indexes of the corresponding infinite system more precisely and economically than other quantities whose use is more standard nowadays. It is the purpose of this paper to illustrate those facts concerning the potential utility of SRO parameters. With that aim we analyse a variety of Monte-Carlo data and study the critical and finite-size scaling properties of SRO.

2. Definitions

For the sake of simplicity, we shall restrict ourselves to the familiar nearest-neighbour spin-$\frac{1}{2}$ ferromagnetic Ising model on a d-dimensional simple (hyper-) cubic lattice with $L^d = N$ lattice sites, and to the corresponding infinite $L \to \infty$ system (see, for instance, Thompson 1972). The main conclusion here, as stated before, should nonetheless hold for more general model systems. Let us denote by n^+, n^-, n^{++}, n^{--}, $n^{+-} = n^{-+}$, respectively, the density (per lattice site) of spins up, spins down, up–up pairs of spins, down–down pairs of spins, and up–down pairs of spins. An appropriate measure of SRO may then be introduced, as in the pioneering studies by Bethe, Rushbrooke, Guggenheim and Fowler (see, for instance, Pathria 1977), as

$$\sigma \equiv \langle n^{++} n^{--} \rangle \langle n^{+-} \rangle^{-2} \tag{2.1}$$

where the brackets represent an average over system configurations at temperature T. Notice that, for all practical purposes, the parameter (2.1) may be assumed to be equivalent to $\sigma' \equiv \langle (n^{++} n^{--})(n^{+-})^{-2} \rangle$, e.g. in the usual case of sharp distributions for n^{++}, etc., neglecting finite-temperature configurations where n^{+-} vanishes. Actually, this is confirmed by some of the data below. In any case, our main conclusions here are independent of that assumption, and one may in practice obtain interesting properties of the phase transition involved either from σ' or else from σ.

Figures 1–4 depict the behaviour of σ, computed by using the Monte Carlo method, as a function of T and, eventually, L in the case of three equilibrium 3D models, namely the pure Ising model (Thompson 1972), the dilute Ising model for several fractions of

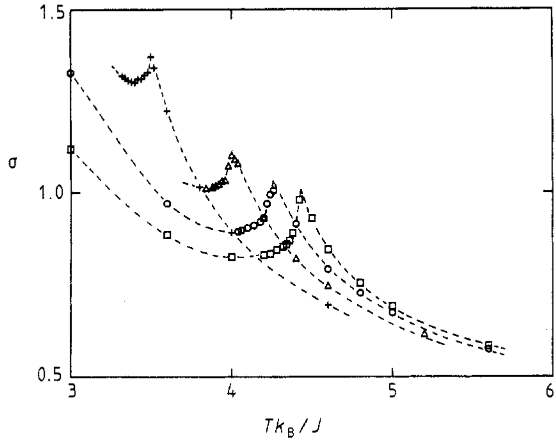

Figure 2. The parameter σ defined in equation (2.1) as a function of temperature in the case of the dilute 3D Ising model (Labarta *et al* 1986) for several concentrations of (non-magnetic) impure sites: $n_0 = 0.0125$ (squares, $L = 30$), 0.05 (open circles, $L = 30$), 0.1 (triangles, $L = 40$), and 0.2 (crosses, $L = 40$).

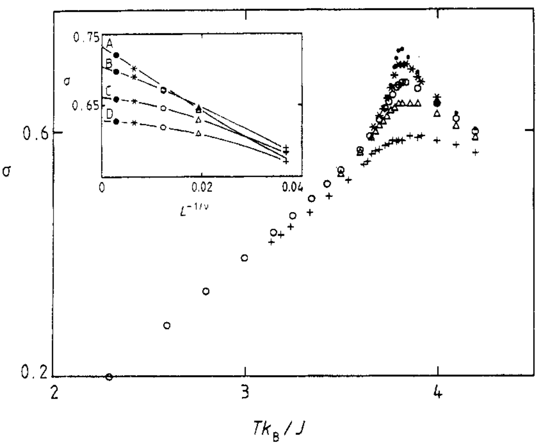

Figure 3. The parameter σ defined in equation (2.1) as a function of temperature in the case of an impure 3D Ising model where 12.5% of the lattice sites, the ones corresponding to a simple cubic sublattice with twice the original lattice spacing, are occupied by spins regularly fixed up, down, up, down, etc., the impure sites producing no net magnetisation (Labarta *et al* 1988). Same symbols as in figure 1. Inset: the dependence of σ on lattice size for temperatures, respectively: $Tk_B/J = 3.79$ (curve A), 3.90 (curve B), 4.00 (curve C) and 3.70 (curve D); $T_c k_B/J = 3.797$ and $\nu = 0.6295$.

non-magnetic sites (Labarta *et al* 1986), and an impure Ising model where 12.5% of spins, regularly distributed on a simple cubic sublattice, are maintained fixed either at $+1$ or else at -1 (instead of allowing each spin to fluctuate between those two values) (Labarta *et al* 1988), and a non-equilibrium, 2D driven-diffusive lattice gas model of fast-ionic conductors (Vallés and Marro 1987), respectively. The qualitative behaviour shown by $\sigma = \sigma(T)$ in those graphs can be understood on simple grounds.

With that aim, it is convenient to relate σ to the system magnetisation and energy. These are given respectively by

$$m \equiv \langle n^+ - n^- \rangle \tag{2.2}$$

and

$$e \equiv -J\langle n^{++} + n^{--} - n^{+-} \rangle = J(2\langle n^{+-} \rangle - d) \tag{2.3}$$

where J (which, for simplicity, is $J > 0$ hereafter) represents the spin interaction strength.

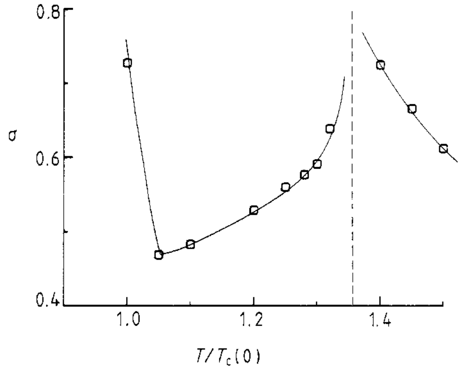

Figure 4. The parameter σ defined in (2.1) as a function of T (in units of the equilibrium critical temperature $T_c(0)$ in the case of a 2D lattice-gas model with attractive interactions and particle-conserving hopping dynamics under the influence of a saturating external electric field along a principal axis (Vallés and Marro 1987). The data refer to the infinite lattice as obtained by extrapolating data for finite systems. The full curve is a guide to the eye; the broken line represents the corresponding critical temperature.

(Notice that e (<0) is a nearest-neighbour correlation function, i.e. it is also a measure of SRO.) Thus, one readily has that

$$\sigma = (1-u)^{-2}[\tfrac{1}{4}(1+u)^2 - m^2] \tag{2.4}$$

where $u \equiv e(T)/e_0$, $1 \geqslant u \geqslant 0$, and $e_0 \equiv -Jd$. The equivalence of expressions (2.1) and (2.4), and the good asymptotic behaviour of the data for finite lattices, is confirmed, for instance, by comparing in figure 1 the Monte Carlo data for $L = 40$, computed according to (2.1), with the corresponding infinite system behaviour obtained from (2.4) after series expansions for u and m (Essam and Fisher 1963, Sykes *et al* 1972, Binder 1972).

3. Further properties of SRO

Expression (2.4) and the definition $\mathrm{d}u/\mathrm{d}T = C_V e_0$ imply that

$$\sigma^{1/2} = (1+u)/2(1-u), \; \mathrm{d}\sigma/\mathrm{d}T = C_V(1+u)/e_0(1-u)^3 \tag{3.1}$$

within the range $m = 0$, i.e. for $T > T_c$. Thus, given that $e_0 < 0$ and $C_V \geqslant 0$, $\sigma(T)$ is expected to decrease monotonically with increasing temperature from maximum value $\sigma_c \equiv \sigma(T_c) > \frac{1}{4}$, in agreement with the situation in figures 1–4. Also, $\sigma(T)$ can only diverge when $T_c = 0$ (the only situation where one could have $u_c \equiv u(T_c) = 1$) and, excluding that case, the fact that $\mathrm{d}\sigma/\mathrm{d}T$ (<0) reaches either a finite or an infinite value at T_c^+ (>0) corresponds respectively to $C_V(T_c^+)$ being finite or infinite. Our data in figures 1–4, which were not specifically produced with that aim and are not very close to T_c^+, hardly allow one to distinguish between those two cases; nevertheless that property may be very useful given both the relevance of the value $C_V(T_c^+)$ to conclude about the nature of a phase transition and the fact that σ can usually be computed more precisely and economically than C_V.

The qualitative differences observed at low temperatures between figure 3, on the one hand, and figures 1, 2 and 4 on the other, are related to the fact that $\langle n^{+-}\rangle$ has a non-zero limit at $T \to 0$ in the case of the impure system in figure 3. Further information for the range $T < T_c$, where $m > 0$, follows from (2.4) and

$$\mathrm{d}\sigma/\mathrm{d}T = (1-u)^{-3}[(1+u-2m^2)(\mathrm{d}u/\mathrm{d}T) - 2m(1-u)(\mathrm{d}m/\mathrm{d}T)]. \tag{3.2}$$

For instance, the situation near T_c^- may be investigated by introducing the asymptotic behaviours $m \sim B\varepsilon^\beta$, $\beta > 0$, and $C_V \sim A\varepsilon^{-\alpha}$, $0 \leqslant \alpha \leqslant 1$, where A and B are both positive and smooth functions of ε, to write,

$$\sigma \sim \sigma_c + a_1\varepsilon^{1-\alpha} - a_2\varepsilon^{2\beta}. \tag{3.3}$$

Here, σ_c is non-singular, and $a_1 \equiv A'(1+u_c)/(1-u_c)^3$, with $A' \equiv -AT_c/(1-\alpha)e_0$, and $a_2 \equiv B^2(1-u_c)^{-2}$ are both positive. It follows immediately that

$$T_c(\mathrm{d}\sigma/\mathrm{d}T) = 2\beta a_2\varepsilon^{2\beta-1} - (1-\alpha)a_1\varepsilon^{-\alpha} \tag{3.4}$$

and one may also work out a similar expression for $\mathrm{d}^2\sigma/\mathrm{d}T^2$.

According to equations (3.3), (3.4) and the corresponding ones for $T \rightarrow T_c^+$, a mean-field behaviour (e.g. $\beta = \frac{1}{2}$, $\alpha = 0$) will be characterised by a smooth variation of $\sigma(T)$ and $\mathrm{d}\sigma/\mathrm{d}T$ near T_c. This is indeed the behaviour shown by the Bethe–Peierls solution of the Ising model (cf. the evidence in figure 4 by Labarta *et al* (1986), for instance). Then, it seems interesting to point out, as a further example of the utility of SRO parameters, that the situation depicted by figure 4 excludes the possibility of the 2D fast-ionic conductor model under a very strong external electric field having a classical critical behaviour; the latter was a conjecture guided by the situation in other non-equilibrium systems (cf Vallés and Marro 1987, Marro *et al* 1987).

In fact, excluding for simplicity the cases (which may also be worked out) where σ decreases or remains constant as $T \rightarrow T_c^-$, the most usual, non-classical critical behaviour is characterised by well-defined maximum around T_c, as in figures 1–4. Thus, the good quality of the data for σ, and the facts that the critical behaviour of σ is mostly dominated by β and that σ_c is finite for $T_c > 0$, should usually allow an easy and accurate computation of T_c and critical indexes. Actually, by using only some limited data at hand we can estimate with little effort that $T_c k_B/J = 4.5108 \pm 0.0001$ and $\beta = 0.312 \pm 0.001$ for the pure 3D Ising model; further specific numerical results are reported below. The investigation of $\sigma(T)$ turns out to be even more convenient given its simple scaling behaviour.

The expected dominant scaling behaviour of σ, as implied by (2.4), (3.3) and usual hypotheses (Barber 1983), is

$$\sigma(\varepsilon, L) - \sigma(0, \infty) - a\varepsilon = L^{-x} f(\varepsilon L^{1/\nu}) \tag{3.5a}$$

where

$$x = \begin{cases} 2\beta/\nu & T < T_c \\ (1-\alpha)/\nu & T > T_c. \end{cases} \tag{3.5b}$$

It follows the same behaviour (3.5*a*) for the energy except that $x = (1-\alpha)/\nu$. That is, one should try to demonstrate that short-range correlation functions scale quite generally according to

$$g(\varepsilon, L) \sim L^{-x} f(\varepsilon L^{1/\nu}) \tag{3.6}$$

with an asymptotic behaviour $f(z) \sim z^x$ for large $z = \varepsilon L^{1/\nu}$ giving the correct exponent x. This is nicely confirmed by figures 5 and 6 revealing the smooth and accurate scaling behaviour of e and σ, respectively, for several interesting lattice systems.

Concerning figure 5, we used $e_c = 0.9921$ as given by series expansions (Sykes *et al* 1972) for the infinite system, and the constant affecting the regular term $a\varepsilon$ was related to the specific heat critical amplitude. That is, we obtain for the latter $-a/T_c = A = -1.24 \pm 0.08$ for $T > T_c$ and -2.44 ± 0.20 for $T < T_c$; both values are in agreement with series (Sykes *et al* 1972) and recent renormalisation group ε-expansions (Chase and Kaufman 1986). It is also noticeable that we only obtain the asymptotic slope $1 - \alpha$ when $A^- = -2.44$ (while the specific heat for the pure Ising model was previously shown (Landau 1976) to scale for $-4 \leqslant A^- \leqslant -2$). The inset in figure 5 is drawn to reveal the unique behaviour when one avoids the sign manipulation and the logarithmic scale in the main graph.

Concerning figure 6, we used $x = 1.41$ for $T > T_c$ and 0.993 for $T < T_c$; this again implies different values for a above and below T_c. The scaling law (3.5) was seen to be valid for all data within the ranges $0.15 \geqslant \varepsilon \geqslant 0$ when $T < T_c$ and $\varepsilon \leqslant -0.005$ when $T > T_c$; the fact that the data for $-0.005 \leqslant \varepsilon \leqslant 0$ in the latter case deviates from scaling is an artefact associated with the hopping of the system very near T_c between $\pm m$ states.

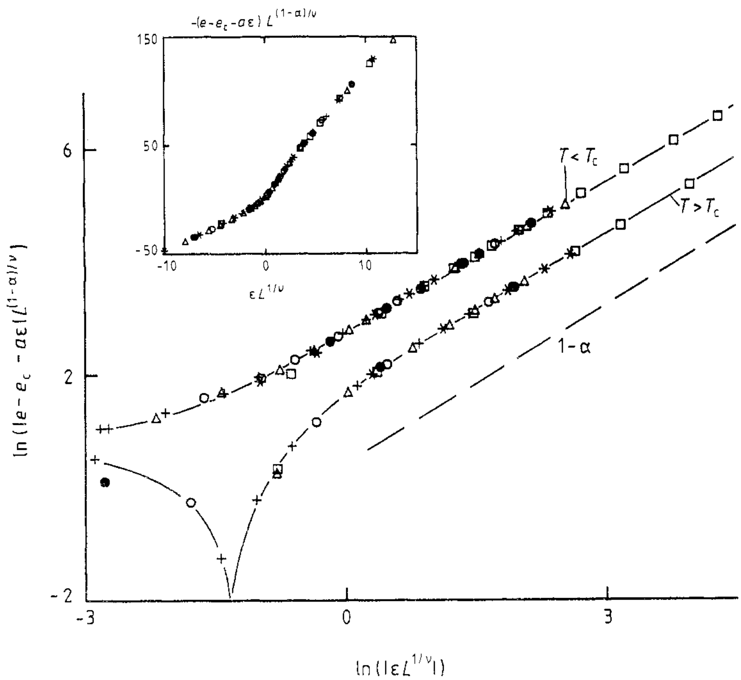

Figure 5. Log-log plot showing the scaling behaviour of the energy e in the case of the pure 3D Ising model; the broken line represents the asymptotic behaviour. Same symbols as in figure 1. Inset: data from which the main graph was plotted.

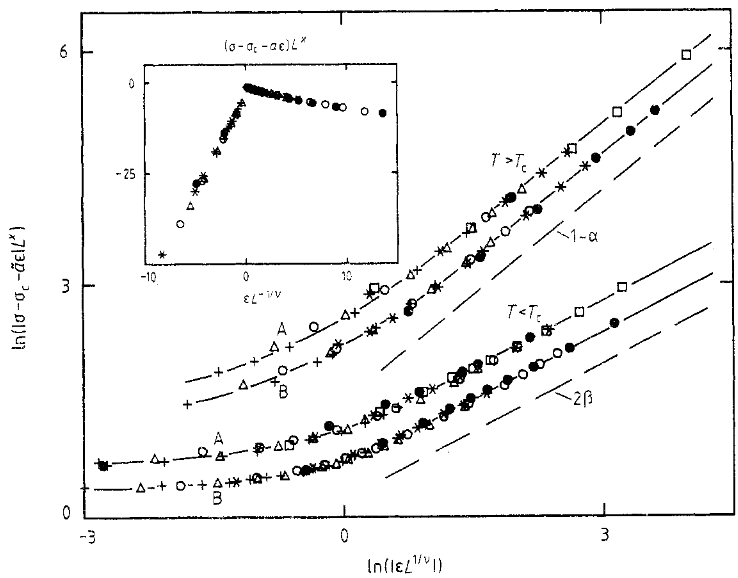

Figure 6. Log-log plot showing the scaling behaviour of the parameter σ, as defined by (2.1), in the cases of the pure system in figure 1 (curves A) and impure system (with fixed spins) in figure 3 (curves B). The behaviour for the system in figure 2 is similar. The broken lines represent the asymptotic behaviour. Inset: data from which the main graph was plotted.

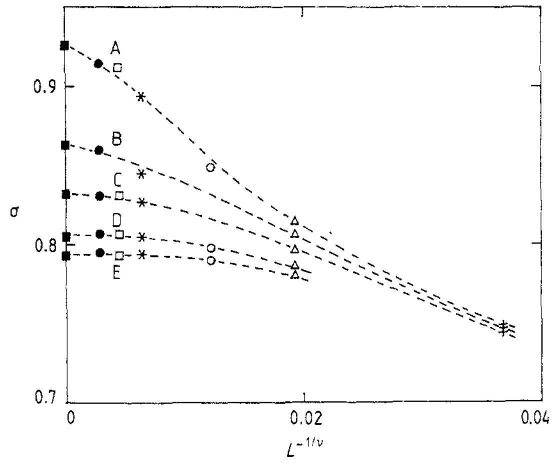

Figure 7. Size dependence of the parameter σ as defined by (2.1) for the pure system in figure 1 when $T < T_c$, namely for $T/T_c = 0.9978$ (curve A), 0.9867 (curve B), 0.9756 (curve C), 0.9534 (curve D) and 0.9313 (curve E). The symbols are for $L =$ 8 (crosses), 12 (open triangles), 16 (open circles), 24 (asterisks), 30 (open squares) and 40 (full circles). The full squares represent σ as given by (2.4).

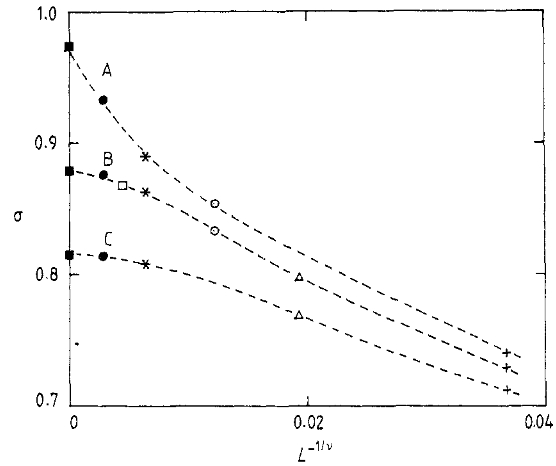

Figure 8. Same as figure 7 but for $T/T_c =$ 1.0022 (curve A), 1.0200 (curve B) and 1.0421 (curve C).

The scaling shown by figure 6 is for $\sigma_c = 0.9882$ (pure system) and 0.764 ± 0.006 (impure system) as obtained from the critical energy values, and for $T_c k_B/J = 4.5108$ (pure) and 3.797 (impure), $\tilde{a}^- = 4 \pm 0.5$ (pure) and 1.5 ± 0.5 (impure), and $\tilde{a}^+ = -11 \pm 1$ (pure), and -8 ± 1 (impure).

Finally, we mention that, as shown by figures 7 and 8 (cf. also figures 1 and 3 for finite-size effects), the most important finite-size effects occur very near T_c, being larger above (figure 8) than below T_c (figure 7). Figures 1–3, 7 and 8 also provide evidence that one may define the temperature $T_c(L)$ locating the maximum of σ rather accurately; this fact should in general allow an easy determination of the critical temperature of the infinite system.

4. Conclusion

The quantity σ defined by (2.1) and, eventually, other SRO parameters possess a number of interesting properties, and they behave more simply and smoothly than other quantities more generally used in the modern theory of phase transitions and critical phenomena. In particular, σ has a simple scaling behaviour with system size, and it usually shows a *finite* and well-defined peak at T_c, whose shape is simply determined by familiar quantities, so that it provides a simple and economical method to evaluate T_c and critical indexes accurately. Moreover, even a visual examination of the behaviour of σ may allow one to distinguish between different universality classes, for instance. Actually, we were able to discard with confidence an expected classical critical behaviour for a fast-ionic conductor model. Those and other properties we suggested above seem indeed to justify the study of SRO parameters when trying to determine, either analytically or numerically (e.g. by Monte Carlo methods), the relevant features of a given phase transition.

Acknowledgments

This work was partially supported by DGICYT (Spain), Project PB85-0062. We also acknowledge data and valuable comments by Lorenzo Vallés in relation to figure 4.

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