Critical dynamics in trapped particle systems

Gianluca Costagliola and Ettore Vicari

Dipartimento di Fisica dell'Università di Pisa and INFN, Sezione di Pisa, Largo Bruno Pontecorvo 2, I-56127 Pisa, Italy

Abstract. We discuss the effects of a trapping space-dependent potential on the critical dynamics of lattice gas models. Scaling arguments provide a dynamic trap-size scaling framework to describe how critical dynamics develops in the large trap-size limit. We present numerical results for the relaxational dynamics of a two-dimensional lattice gas (Ising) model in the presence of a harmonic trap, which support the dynamic trap-size scaling scenario.

Statistical systems are generally inhomogeneous in nature, while homogeneous systems are often an ideal limit of experimental conditions. Critical phenomena, characterized by the development of correlations with diverging length and time scales, are usually considered assuming homogeneous systems. However, the emergence of critical correlations is also observed in inhomogeneous systems. Particularly interesting physical systems are interacting particles constrained within a limited region of space by an external potential. This is a common feature of the experimental realizations of Bose-Einstein condensations in diluted atomic vapors [1] and of optical lattices of cold atoms [2]. Experimental evidence [3] of a critical behavior has been reported for a three-dimensional trapped Bose gas, observing an increasing correlation length compatible with a continuous transition, although the system is made inhomogeneous by the confining force. Experimental evidences of finite-T Kosterlitz-Thouless transitions [4] in two-dimensional trapped Bose atomic gases have been provided in [5, 6, 7, 8, 9]. However, the inhomogeneity due to the trapping potential is expected to strongly affects the phenomenology of continuous phase transitions observed in the absence of a trap. For example, correlation functions of the critical modes are not expected to develop a diverging length scale in a trap. Therefore, a theoretical description of the critical correlations in systems subject to confining potentials, and of how they unfold approaching the transition point, is of great importance for experimental investigations of the critical behavior of systems of trapped interacting particles.

We consider a trapping potential

$$V(r) = v^p|\vec{r}|^p \equiv (|\vec{r}|/l)^p, \tag{1}$$

where v and p are positive constants and $l = v^{-1}$ is the *trap size*, coupled to the particle number. Harmonic potentials, i.e., $p = 2$, are usually realized in experiments. The effect of the trapping potential is to effectively vary the local value of the chemical potential, so that the particles cannot run away. Let us consider the case in which the system parameters, such as temperature, pressure and chemical potential, are tuned to values corresponding to the critical regime of the unconfined system. The critical behavior gets distorted by the trap, although it gives rise to universal effects in the large trap-size limit, controlled by the universality class of the phase transition of the unconfined system. The corresponding scaling regime can be cast in the form of a trap-size scaling (TSS) [10, 11], resembling the finite-size scaling theory for homogeneous systems, but characterized by a further nontrivial *trap* critical exponent θ, which describes how the length scale ξ of the critical modes depends on the trap size at criticality, i.e., $\xi \sim l^\theta$, and which can be estimated using renormalization-group (RG) arguments.

In this paper we investigate how critical dynamics develop in trapped systems at thermal continuous transitions, i.e., *classical* transition driven by thermal fluctuations. We extend the TSS Ansatz of [10], to allow for the time dependence of the critical modes, which depends on the static universality class, but also on the general features of the dynamics, analogously to homogeneous systems [12].

In a standard scenario for a continuous transition, see, e.g., [13], the critical behavior of a d-dimensional system is characterized by two relevant parameters u_t and u_h, which may be associated with the temperature T, i.e., $u_t \sim T/T_c - 1$, and the external field h coupled to the order parameter, whose RG dimensions are $y_t = 1/\nu$ and $y_h = (d+2-\eta)/2$. The presence of a trap of size l generally induces a further length scale $\xi_{\rm trap} \sim l^\theta$, which must be taken into account to describe the critical correlations. Within the TSS framework [10, 11], see also [14, 15, 16, 17, 18, 19, 20, 21, 22], the scaling law of the singular part of the free energy density around the center of the trap can be written as

$$F_{\rm sing} = l^{-\theta d} \mathcal{F}(u_t l^{\theta y_t}, u_h l^{\theta y_h}, x l^{-\theta}) \tag{2}$$

where θ is the *trap exponent*. At the critical point $u_t = 0$, the TSS of the correlation function of the order parameter ϕ is

$$G(x,y) \equiv \langle \phi(x)\phi(y)\rangle_c = l^{-\theta(d-2+\eta)} f(x l^{-\theta}, y l^{-\theta}), \tag{3}$$

thus implying $\xi \sim l^\theta$ for its length scale. Finite size effects, due to a finite volume L^d, can be taken into account by adding a further dependence on $L l^{-\theta}$ in the above scaling Ansatz [19].

The universal scaling behavior of the critical dynamics is essentially determined by the dynamic universality class, which depends on a few general properties of the dynamics, for example, whether there are conserved quantities during the time evolution (see [12] for a list of dynamic universality classes). The scaling behavior of the correlation functions requires a further dynamic critical exponent z, which provides the power-law relation between the critical time scale τ and the diverging correlation length $\tau \sim \xi^z \sim u_t^{-z\nu}$, thus implying a diverging time scale at the critical point. For example, the equilibrium time dependence of the correlation function of the order parameter $\phi(x,t)$ is expected to scale as

$$G(x_1,x_2;t_1,t_2) \equiv \langle \phi(x_1,t_1)\phi(x_2,t_2)\rangle_c = \xi^{-(d-2+\eta)} f[(x_2-x_1)/\xi, (t_2-t_1)/\xi^z] \tag{4}$$

Again, the presence of the trap drastically affects the critical dynamics; in particular, the time correlations are not expected to develop a diverging time scale. Within the TSS framework, the time dependence of the dynamic scaling behavior is expected to enter through a further dependence on the scaling variable $tl^{-\theta z}$. Thus, at the critical point $u_t = 0$, the scaling behavior at equilibrium of the two-point correlation function (4) is expected to be

$$G(x_1, x_2; t_1, t_2) = l^{-\theta(d-2+\eta)} f_g[x_2 l^{-\theta}, x_1 l^{-\theta}, (t_2 - t_1) l^{-\theta z}] \tag{5}$$

which implies that the corresponding time scale τ behaves as

$$\tau \sim l^{\theta z} \tag{6}$$

at the critical point. Analogous scaling behaviors have been put forward to describe the temperature and time dependence at $T = 0$ quantum transitions [11, 23, 24]. The dynamic TSS Ansatz can also be extended to take into account off-equilibrium dynamics.

In order to check the dynamic TSS scenario, we consider the lattice gas model defined by the Hamiltonian

$$\mathcal{H}_{\rm Lgas} = -4J \sum_{\langle ij \rangle} \rho_i \rho_j - \mu \sum_i \rho_i + \sum_i 2V(r_i)\rho_i \tag{7}$$

where the first sum runs over the nearest-neighbor sites of a square lattice, $\rho_i = 0, 1$ depending if the site is empty or occupied by the particles, μ is the chemical potential, and $V(r)$ is the potential (1) which vanishes at the center of the trap. Far from the origin the potential diverges, thus the expectation value of the particle number tend to vanish, indeed $\langle \rho_x \rangle \sim \exp[-2V(x)]$ at large distance from the center, and therefore the particles are trapped. The lattice gas model (7) can be exactly mapped to a standard Ising model, by replacing $\rho_i = (1 - s_i)/2$, obtaining

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i - \sum_i V(r_i) s_i \tag{8}$$

where $s_i = \pm 1$ and $h = 8J + \mu/2$. In this picture the external potential plays the role of a space-dependent magnetic field. In the absence of the trap, the square-lattice Ising model (8) shows a critical behavior characterized by the critical exponents $\nu = 1$ and $\eta = 1/4$, at the critical point $T = T_c = 2/\ln(\sqrt{2} + 1)$ (we set $J = 1$) and $h = h_c = 0$. Critical correlations do not develop a diverging length scale in the presence of the external space-dependent potential, i.e., at fixed $v > 0$. But a critical behavior develops in the limit $v \to 0$, described by TSS as in Eqs. (2) and (3). The trap exponent is given by

$$\theta = 16/31, \tag{9}$$

which can be derived by RG scaling arguments [10] taking into account the fact that the external potential couples to the order parameter. The static TSS has been numerically investigated in [10], here we focus on the dynamic TSS scenario of Eqs. (5) and (6).

We consider a purely relaxational dynamics (also known as model A of critical dynamics [12]), which can be realized by Metropolis updatings in Monte Carlo simulations. The corresponding dynamic exponent z has been accurately determined in homogeneous systems by numerical equilibrium and off-equilibrium methods, obtaining $z \approx 2.17$. ‡ According to the dynamic TSS scenario, in the presence of the trap we should not observe any diverging time scale τ, but the critical dynamics is only recovered in the limit $l \to \infty$, with a power-law diverging time scale (6).

In our simulations we consider square lattices with $-L \le x, y \le L$, and trap potential $V(x) = (x^2 + y^2)/l^2$ (thus the trap is centered at the origin), while at the boundaries $|x|, |y| = L + 1$ the spin variable is kept fixed: $s_i = 1$ (corresponding to $\rho_i = 0$). In the presence of the trap of size l, the lattice size L is chosen to have the spin variables effectively frozen at the boundary, making unnecessary the use of larger lattices to effectively obtain infinite volume results. See also below. The dynamics is provided by Metropolis updatings of the lattice variables using a checkerboard scheme (a time unit corresponds to a sweep of the lattice). We present results of MC simulations for several values of the trap size, up to $l = 320$. The typical statistics of our simulations is 10^9 sweeps.

We want to determine the power-law behavior of the time scale at $T = T_c$ as a function of the trap size. For this purpose we estimate the autocorrelation times of the magnetization along the lattice axes, which can be easily computed. More precisely, we define

$$M_r \equiv \sum_{i=-\lfloor rl^\theta \rfloor}^{\lfloor rl^\theta \rfloor} s_{i0} + s_{0i} \tag{10}$$

where $\lfloor x \rfloor \equiv \text{floor}(x)$ is the largest integer not greater than x, the distance r is measured in unit of the length scale l^θ (to construct nonlocal observables compatible with the expected TSS behavior), and the subscripts of s_{ij} indicate the coordinate of the lattice sites. In the following analysis we consider the values $r = 1/2$ and $r = 1$. We estimate the autocorrelation times of the correlators

$$C_r(t_2 - t_1) = \langle M_r(t_1) M_r(t_2) \rangle_c \tag{11}$$

For this purpose we exploit the method of [35] which provides a substantial numerical advantage because it does not require extrapolated large-time estimates of the autocorrelation functions. We define

$$\hat{\tau}_r(t + n/2) \equiv \frac{n}{\ln[C_r(t)/C_r(t+n)]}, \tag{12}$$

where n is a fixed integer number. A linear interpolation can be used to extend $\hat{\tau}_r(t)$ to all real numbers. Then, for any positive x, we define an autocorrelation time $\tau_{r,x}$ as the

‡ Some of the most recent equilibrium estimates are $z = 2.1667(5)$ from [25], $z = 2.168(5)$ from [26], $z = 2.1665(12)$ from [27], $z = 2.172(6)$ from [28]. Off-equilibrium results are $z = 2.156(2)$ from [29], $z = 2.153(2)$ from [30], $z = 2.16(3)$ from [31], $z = 2.1337(41)$ from [32], $z = 2.160(5)$ from [33], $z = 2.165(10)$ from [34]. The apparent small discrepancy between the two sets of results should not be significant.

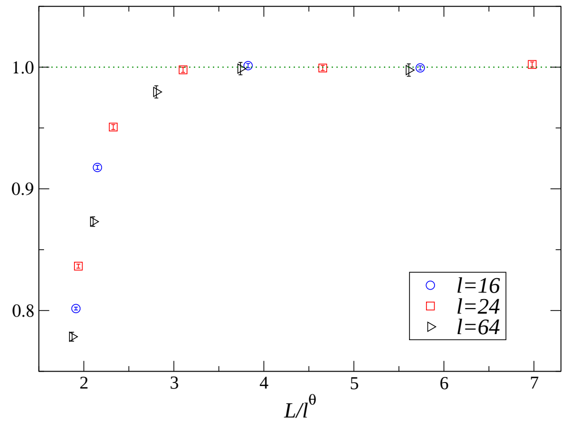

Figure 1. The ratio $\tau_{1/2}(L)/\tau_{1/2}(\infty)$ vs $Ll^{-\theta}$.

solution of the equation §

$$\tau_{r,x} = \hat{\tau}_r(x\tau_{r,x}). \tag{13}$$

$\tau_{r,x}$ are expected to show the same power-law behavior with increasing l, i.e., $\tau_{r,x} \sim l^{\kappa}$. After some checks, we chose $x = 2$ as optimal value for our calculations, so in the following we present only results for $x = 2$ and skip the subscript indicating the value of x.

Let us first discuss the finite size effects due to a finite volume L^2, which are expected to enter through the FSS variable $Ll^{-\theta}$ [19]. This is confirmed by Fig. 1, which shows the data of the ratio $\tau_{1/2}(L)/\tau_{1/2}(\infty)$ between the autocorrelation times of $M_{1/2}$ at a given L and in the $L \to \infty$ limit, as estimated by the result for the largest available lattice. The analysis of the FSS effects show that, within an accuracy of a few per mille, the data for $Ll^{-\theta} \gtrsim 5$ can be effectively considered as $L \to \infty$ data.

In Fig. 2 we show the resulting infinite-volume estimates of the autocorrelation times of $M_{1/2}$ and M_1, up to a trap size $l = 320$. They clearly show an asymptotic power-law behavior. The data for $l \geq 48$ turn out to fit the simple power law $\tau_r = al^{\kappa}$ with $\chi^2/\text{d.o.f} \lesssim 1$, providing the estimate $\kappa = 1.120(3)$ (the results of the fits appear reasonably stable with increasing the minimum value of l allowed in the fit, while the data for $l < 48$ show small deviations from the simple power law). Analogous results are obtained by varying the value of x in the definition (13). Dividing the exponent κ by $\theta = 16/31$, we obtain

$$\kappa/\theta = z = 2.170(6) \tag{14}$$

which is in good agreement with the best available estimates of z, for example [25] $z = 2.1667(5)$. We have also performed fits to all data including scaling corrections, which are expected to be [11] $O(l^{-\theta})$, obtaining consistent results.

§ This definition is based on the idea that, if the autocorrelation function $C(t)$ were a pure exponential, i.e., $C(t) = C_0 \exp(-t/\tau)$, then $\hat{\tau}(t) = \tau$ for all t and thus $\tau_x = \tau$ for any x. It provides a good autocorrelation time for any x, which converges to the integrated autocorrelation time $\tau_{\rm int} = \frac{1}{2}\sum_{t=-\infty}^{\infty} C(t)/C(0)$ for $x \to \infty$. See [35] for a through discussion.

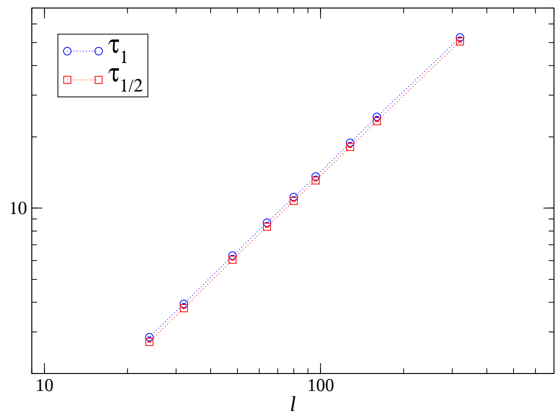

Figure 2. Power-law behavior of the autocorrelation times $\tau_{1/2}$ and τ_1. The lines are drawn to guide the eyes.

In conclusion, our numerical results for the relaxational dynamics of the square-lattice gas model (7) show that the dynamic TSS scenario correctly describes the development of a critical dynamics in the presence of an inhomogeneous external potential which acts as a trap for particle systems. We expect that the validity of the dynamic TSS extends to other dynamic universality classes.

References

[1] Cornell E A and Wieman C E, 2002 *Rev. Mod. Phys.* **74** 875; Ketterle N, 2002 *Rev. Mod. Phys.* **74** 1131
[2] Bloch I, Dalibard J, and Zwerger W, 2008 *Rev. Mod. Phys.* **80** 885
[3] Donner T, Ritter S, Bourdel T, Öttl A, Köhl M, and Esslinger T, 2007 *Science* **315** 1556
[4] Kosterlitz J M and Thouless D J, 1973 *J. Phys. C: Solid State* **6** 1181
[5] Hadzibabic Z, Krüger P, Cheneau M, Battelier B, and Dalibard J, 2006 *Nature* **441** 1118.
[6] Krüger P, Hadzibabic Z, and Dalibard J, 2007 *Phys. Rev. Lett.* **99** 040402
[7] Hadzibabic Z, Krüger P, Cheneau M, Rath S P, and Dalibard J, 2008 *New J. Phys.* **10** 045006
[8] Cladé P, Ryu C, Ramanathan A, Helmerson K, and Phillips W D, 2009 *Phys. Rev. Lett.* **102** 170401
[9] Hung C-L, Zhang X, Gemelke N, and Chin C, 2011 *Nature* **470** 236
[10] Campostrini M and Vicari E, 2009 *Phys. Rev. Lett.* **102** 240601; 2009 *Phys. Rev. Lett.* **103** 269901 (E)
[11] Campostrini M and Vicari E, 2010 *Phys. Rev.* A **81** 023606; 2010 *Phys. Rev.* A **81** 063614
[12] Hohenberg P C and Halperin B I, 1977 *Rev. Mod. Phys.* **49** 435
[13] Pelissetto A and Vicari E, 2002 *Phys. Rept.* **368** 549
[14] Burkhardt T W, 1982 *Phys. Rev. Lett.* **48** 216
[15] Platini T, Karevski D, and Turban L, 2007 *J. Phys. A: Math. Theor.* **40** 1467
[16] Zurek W H and Dorner U, 2008 *Phyl. Trans. R. Soc.* A **366** 2953
[17] Eisler V, Iglói F and Peschel I, 2009 *J. Stat. Mech.* P02011
[18] Collura M, Karevski D, and Turban L, 2009 *J. Stat. Mech.* P08007
[19] de Queiroz S L A, dos Santos R R, and Stinchcombe R B, 2010 *Phys. Rev.* E **81** 051122
[20] Pollet L, Prokof'ev N V, and Svistunov B V, 2010 *Phys. Rev. Lett.* **104** 245705
[21] Campostrini M and Vicari E, 2010 *J. Stat. Mech.* P08020
[22] Crecchi F and Vicari E, 2011 *Phys. Rev.* A **83** 035602
[23] Collura M and Karevski D, 2010 *Phys. Rev. Lett.* **104** 200601

[24] Campostrini M and Vicari E, 2010 *Phys. Rev.* A **82** 063636
[25] Nightingale M P and Blöte H W J, 2000 *Phys. Rev.* B **62** 1089
[26] Wang F-G and Hu C-K, 1997 *Phys. Rev.* E **56** 2310
[27] Nightingale M P and Blöte H W J, 1996 *Phys. Rev. Lett.* **76** 4548
[28] Grassberger P, 1995 *Physica* A **214** 547
[29] Da Silva R, Alves N A, and de Felicio J D, 2002 *Phys. Lett.* A **298** 325
[30] Zhang J B, Wang L, Gu D-W, Ying H-P, and Ji D-R, 1996 *Phys. Lett.* A **262** 226
[31] Soares M S, Leal da Silva J K, and Sa Barreto F C, 1996 *Phys. Rev.* B **55** 1021
[32] Li Z B, Schulke L, and Zheng B, 1995 *Phys. Rev. Lett.* **74** 3396
[33] Linke A, Heerman D W, Altevogt P, and Siegert M, 1995 *Physica* A **222** 205
[34] Ito N, 1993 *Physica* A **196** 591
[35] Hasenbusch M, Pelissetto A, and Vicari E, 2007 *J. Stat. Mech.* P11009