Journal of Statistical Physics, Vol. 31, No. 2, 1983

Critical-Point Limit Law for Temperley's Continuous Model

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Received June 2, 1982; revised November 4, 1982

We consider the probability distribution of the volume V_N in a N-particle Temperley's model of liquid–gas condensation. We rigorously prove that the critical-point limit law of $(V_N - Nv_c)/N^{3/4}$ exists and has probability density proportional to $\exp(-cx^4)$ $(c > 0)$. This result shows that the probabilistic approach to critical phenomena may be extended to continuous fluid systems.

KEY WORDS: Limit laws; Temperley's model.

1. INTRODUCTION

In the probabilistic approach to the renormalization group[1,2] one usually studies the limit law of $M_N/N^{\rho/2}$ where M_N is the random variable associated to the magnetization of a system of N spins; the index ρ is to be chosen such that the critical-point limit law exists. It is well known that this procedure may be extended to other systems such as the lattice gas and Euclidian field theories. The main advantage of this formulation is to give a precise meaning to the notion of universality classes: any model characterized by the same limit law should provide the same critical exponents. Up to now, two examples have been rigorously treated: the first by Ellis and Newman[3,4] (Curie–Weiss) and the second by Abraham[5] (edge of an Ising model). A program for a general theory has recently been proposed by Newman[6] but only for magnetic substances. In the same way that Wilson's approach can be applied to liquid–gas systems,[7] it would be interesting to extend this probabilistic point of view to continuous fluid models.

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We rigorously prove in this paper that such a probabilistic approach (which has already been successfully applied to classical magnetic models[11]) may be extended to Temperley's model of condensation. We consider the random variable V_N associated to the volume of a N-particle system and establish the existence of the critical-point limit law of $(V_N - Nv_c)/N^{3/4}$ as $N \to +\infty$. The analysis is carried over in the pressure ensemble which ensures that this limiting procedure is equivalent to the thermodynamic limit.[4] Proofs of the lemmas used in the Section 2 are to be found in Section 3.

2. THE LIMIT LAW OF THE VOLUME FOR TEMPERLEY'S MODELS

Let us consider N hard-core particles in a volume V under the assumption of nonoverlapping covolumes v_0. We write N^2a/V for the attractive potential energy of the system. The partition function in the canonical ensemble takes the form

$$Z(T,V,N) = \frac{e^{\beta N^2 a/V}}{\lambda^{3N}} \frac{1}{N!} V(V-v_0)\cdots\left[V-(N-1)v_0\right] \quad (2.1)$$

This is Temperley's cell model which amounts to dividing the volume V into elementary cells of volume v_0 occupied at most by a single particle. Going over to the (T,P,N) ensemble enables one to compute the probability density of the volume in a system with fixed inverse temperature β, pressure P and number of particles N. Let f_{V_N} be this density:

$$f_{V_N}(V) = \frac{e^{-\beta PV}\partial_V Z(T,V,N)}{Y(T,P,N)} \quad (2.2)$$

where $Y(T,P,N)$ is the partition function in the pressure ensemble:

$$Y(T,P,N) = \beta P \int_{Nv_0}^{+\infty} e^{-\beta PV} Z(T,V,N)\,dV \quad (2.3)$$

The substitution $V = Nv$ leads to the following form of the density (2.2):

$$f_{V_N}(Nv) = \frac{e^{-\beta PNv}\partial_{Nv}\left[e^{\beta Na/v}G_N(v/v_0)\right]}{N\beta PD_N(\beta,P)} \quad (2.4)$$

with

$$D_N(\beta,P) = \int_{v_0}^{+\infty} e^{-\beta PNv+\beta Na/v} G_N\left(\frac{v}{v_0}\right) dv \quad (2.5)$$

and

$$G_N(z) = \prod_{i=0}^{N-1}\left(z - \frac{i}{N}\right) \quad (2.6)$$

We shall also use the following notations:

$$\Pi(v) = -\frac{1}{v_0}\ln\left(1 - \frac{v_0}{v}\right) - \frac{a\beta}{v^2} \tag{2.7}$$

$$h(v) = \beta P v - \beta\frac{a}{v} - \frac{v}{v_0}\ln\frac{v}{v_0} + \left(\frac{v}{v_0} - 1\right)\ln\left(\frac{v}{v_0} - 1\right) \tag{2.8}$$

In order to show that the limit probability distribution of the suitably renormalized random variable V_N exists when $N \to +\infty$, we shall first construct upper and lower bounds for the density (2.4).

Lemma 1. For any positive real number m and any v/v_0 belonging to $[1 + 1/m, +\infty[$, we have the following inequalities:

$$-\frac{m^2}{2Nv_0} \leqslant \partial_{Nv}\ln\left[e^{\beta N a/v}G_N\left(\frac{v}{v_0}\right)\right] - \Pi(v) < 0 \tag{2.9}$$

and

$$\exp\left\{-N\left[h(v) + 1\right] - \frac{1}{2}\ln\left(1 - \frac{v}{v_0}\right) - \frac{m^2}{4N}\right\}$$
$$< \exp\left(-\beta P N v + \beta\frac{Na}{v}\right)G_N\left(\frac{v}{v_0}\right) \tag{2.10a}$$

$$\exp\left\{-N\left[h(v) + 1\right] - \frac{1}{2}\ln\left(1 - \frac{v_0}{v}\right) + \frac{m^2}{6N}\right\}$$
$$> \exp\left(-\beta P N v + \beta\frac{Na}{v}\right)G_N\left(\frac{v}{v_0}\right) \tag{2.10b}$$

Combining (2.9) and (2.10) with the expression (2.4) for the density $f_{V_N}(Nv)$ we obtain if $v/v_0 \geqslant 1 + 1/m$

$$f_{V_N}(Nv) > \frac{\exp\left\{-\frac{m^2}{4N} - N\left[h(v) + 1\right] - \frac{1}{2}\ln\left(1 - \frac{v_0}{v}\right)\right\}\left[\Pi(v) - m^2/2Nv_0\right]}{N\beta P D_N(\beta, P)} \tag{2.11}$$

and

$$f_{V_N}(Nv) < \frac{\exp\left\{\frac{m^2}{6N} - N\left[h(v) + 1\right] - \frac{1}{2}\ln\left(1 - \frac{v_0}{v}\right)\right\}}{N\beta P D_N(\beta, P)}\Pi(v) \tag{2.12}$$

Let us write $P\{Na < V_N \leqslant Nb\}$ for the probability that the volume takes a value between Na and Nb $(v_0 < a < b)$:

$$P\{Na < V_N \leqslant Nb\} = \int_{Na}^{Nb} f_{V_N}(V)\,dV \tag{2.13}$$

In order to study the behavior of this probability at the critical point, we construct the renormalized variable $(V_N - Nv_c)/N^{3/4}$ at $\beta = \beta_c$ and $P = P_c$. These critical parameters of the system are easily derived from the equation of state (2.7)[9,10]:

$$v_c = 2v_0, \qquad \beta_c = \frac{2v_0}{a}, \qquad P_c = \frac{a}{v_0^2}\ln\left|\sqrt{2} - \frac{1}{4}\right| \tag{2.14}$$

Equations (2.11) and (2.13) lead to

$$\begin{aligned} P\left\{A < \frac{V_N - Nv_c}{N^{3/4}} \leqslant B\right\} \\ > \Bigg[\exp\left(-\frac{m^2}{4N} - N\right) \\ \cdot N^{3/4}\int_A^B dx\,\Bigg\{\exp\left[-Nh_c\left(\frac{x}{N^{1/4}} + v_c\right) - \frac{1}{2}\ln\left(1 - \frac{v_0}{x/N^{1/4} + v_c}\right)\right] \\ \times\left[\Pi_c\left(\frac{x}{N^{1/4}} + v_c\right) - \frac{m^2}{2Nv_0}\right]\Bigg\}\Bigg] \Big/ N\beta_c P_c D_N(\beta_c, P_c) \end{aligned} \tag{2.15}$$

where A and B are fixed real numbers and where N is to be chosen such that $-N^{1/4}(1 - 1/m)v_0 \leqslant A < B$. (This restriction on N ensures that $v/v_0 \geqslant 1 + 1/m$ for any real A and B.) In (2.15) as well as in what follows the subscript c denotes the value of the corresponding function at (β_c, P_c). In the same way we obtain from (2.12) and (2.13)

$$\begin{aligned} P\left\{A < \frac{V_n - Nv_c}{N^{3/4}} \leqslant B\right\} \\ \leqslant \Bigg[e^{m^2/6N - N} \\ \cdot N^{3/4}\int_A^B dx\,\Bigg\{\exp\left[-Nh_c\left(\frac{x}{N^{3/4}} + v_c\right) - \frac{1}{2}\ln\left(1 - \frac{v_0}{x/N^{1/4} + v_c}\right)\right] \\ \times \Pi_c\left(\frac{x}{N^{1/4}} + v_c\right)\Bigg\}\Bigg] \Big/ n\beta_c P_c D_N(\beta_c, P_c) \end{aligned} \tag{2.16}$$

We now show that for $N \to +\infty$ the lower bound (2.15) becomes equal to the upper one (2.16).

Lemma 2. For any N such that $-N^{1/4}(1-1/m)v_0 \leqslant A < B$, there exist real numbers z_1, z_2, $(z_1 \leqslant z_2)$, w_1, w_2 $(w_1 \leqslant w_2)$ and y_1, y_2 $(y_1 \leqslant y_2)$ such that for any x belonging to $[A, B]$, we have

$$\frac{z_1}{N^{1/4}} \leqslant Nh_c\left(\frac{x}{N^{1/4}} + v_c\right) - Nh_c - \frac{1}{4!}x^4 h_c^{(4)}(v_c) \leqslant \frac{z_2}{N^{1/4}} \tag{2.17}$$

$$\frac{w_1}{N^{3/4}} \leqslant \Pi_c\left(\frac{x}{N^{1/4}} + v_c\right) - \beta_c P_c \leqslant \frac{w_2}{N^{3/4}} \tag{2.18}$$

and

$$\frac{y_1}{N^{1/4}} \leqslant \frac{1}{2}\ln\left(1 - \frac{v_0}{x/N^{1/4} + v_c}\right) + \ln\sqrt{2} \leqslant \frac{y_2}{N^{1/4}} \tag{2.19}$$

where $h_c = h_c(v_c)$.

With the help of this lemma we may rewrite the inequalities (2.15) and (2.16) as

$$P\left\{A < \frac{V - Nv_c}{N^{3/4}} \leqslant B\right\}$$

$$> \frac{\exp\left(-\frac{m^2}{4N} - \frac{z_2 + y_2}{N^{1/4}} + \ln\sqrt{2}\right)\left[N^{3/4}\left(\beta_c P_c - \frac{m^2}{2Nv_0}\right) + w_1\right] \times \int_A^B dx \exp\left[-\frac{1}{4!}x^4 h_c^{(4)}(v_c)\right]}{Ne^{N[h_c+1]}\beta_c P_c D_N(\beta_c, P_c)} \tag{2.20a}$$

$$P\left\{A < \frac{V_N - Nv_c}{N^{3/4}} \leqslant B\right\}$$

$$< \frac{\exp\left(\frac{m^2}{6N} - \frac{z_1 + y_1}{N^{1/4}}\right)\left(N^{3/4}\beta_c P_c + w_2\right)\int_A^B dx \exp\left[-\frac{1}{4!}x^4 h_c^{(4)}(v_c)\right]}{N\beta_c P_c e^{N[h_c+1]} D_N(\beta_c, P_c)} \tag{2.20b}$$

The reduction of the normalization factor is made possible by using the following lemmas:

Lemma 3. For any $0 < p < 1$, we have

$$0 < \exp\left[N(h_c + 1)\right] \int_{v_0}^{v_0(1+p)} dv \exp\left(-\beta_c P_c N v + \beta_c \frac{a}{v} N\right) G_N\left(\frac{v}{v_0}\right)$$
$$< (N+1) p v_0 \exp\left\{1 - N\left[h_c(v_0(1+p)) - h_c\right]\right\} \tag{2.21}$$

[Let us remark that $h_c(v)$ being minimum at v_c, the upper bound tends to zero for $N \to +\infty$.]

Lemma 4. For any $0 < \mu < |n(v_c)|$, $[n(v_c) = -(1/4!) h_c^{(4)}(v_c) < 0]$ and any $0 < p < 1$, we may find positive real numbers δ, $n(\delta)$ and $\alpha(\delta, \mu)$ such that for $N > 1$

$$e^{Nh_c} \int_{v_0(1+p)}^{+\infty} e^{-Nh_c(v)} \frac{dv}{(1 - v_0/v)^{1/2}}$$
$$> \frac{ck(\delta)}{\left[N|n(v_c) - \mu|\right]^{1/4}} \left[1 - N^{1/4} e^{-(N-1)\alpha(\delta,\mu)}\right] \tag{2.22a}$$

and

$$e^{Nh_c} \int_{v_0(1+p)}^{+\infty} e^{-Nh_c(v)} \frac{dv}{(1 - v_0/v)^{1/2}}$$
$$< L(p) e^{-(N-1)\eta(\delta)} + \frac{ck(-\delta)}{\left[N|n(v_c) + \mu|\right]^{1/4}} \tag{2.22b}$$

and

$$k(x) \equiv \left(\frac{x + 2v_0}{x + v_0}\right)^{1/2} \tag{2.23}$$

We write $D_N(\beta_c, P_c)$ under the form

$$D_n(\beta_c, P_c) = \left(\int_{v_0}^{v_0(1+p)} + \int_{v_0(1+p)}^{+\infty}\right) dv \exp\left(-\beta P N v + \beta \frac{Na}{v}\right) G_N\left(\frac{v}{v_0}\right) \tag{2.24}$$

For $N \to +\infty$, the contribution of the first integral in (2.24) to (2.20) tends to zero. Using (2.10) in the evaluation of the second integral, the combination of (2.20), (2.22), and the definition (2.23) lead when $\mu \to 0$ to the limit law:

Theorem. For any real numbers A and B and with the previously defined notations

$$\lim_{N\to+\infty} P\left\{A < \frac{V_N - Nv_c}{N^{3/4}} \leqslant B\right\} = \frac{|n(v_c)|^{1/4}}{c} \int_A^B dx\, e^{-x^4|n(v_c)|} \tag{2.25}$$

This result is quite general as it does not depend on the value of m [see remark after Eq. (2.15)].

This limit law has already been obtained for magnetic substances in the Curie–Weiss model.[4,11] According to the probabilistic formulation of the universality classes of critical phenomena, we expect identical critical-point exponents. That this is true[12] provides a nice illustration of the connection between limit laws and universality. Studying the domain of attraction of the limit law $\exp(-cx^4)$ will provide a nice approach to a general mean-field approximation.

3. PROOFS OF THE LEMMAS

Proof of Lemma 1. Relation (2.9) may be written in the following form:

$$-\frac{m^2}{2Nv_0} \leqslant \partial_{Nv}\ln\left[G_N\left(\frac{v}{v_0}\right)\right] + \frac{1}{v_0}\ln\left(1 - \frac{v_0}{v}\right) < 0 \tag{3.1}$$

Let

$$f(x) = \ln(z - x) \qquad \text{with} \quad z = v/v_0 \tag{3.2}$$

From the definition (2.6) we have

$$\ln G_N(z) = \sum_{i=0}^{N-1} f\left(\frac{i}{N}\right) \tag{3.3}$$

and therefore

$$\partial_{Nv}\ln G_N\left(\frac{v}{v_0}\right) = -\frac{1}{Nv_0}\sum_{i=0}^{N-1} f^{(1)}\left(\frac{i}{N}\right) \tag{3.4}$$

On the other hand

$$\ln\left(1 - \frac{v_0}{v}\right) = f(1) - f(0) = \int_0^1 f^{(1)}(x)\,dx \tag{3.5}$$

so that

$$-\frac{m^2}{2N} \leqslant -\frac{1}{N}\sum_{i=0}^{N-1} f^{(1)}\left(\frac{i}{N}\right) + \int_0^1 f^{(1)}(x)\,dx < 0 \tag{3.6}$$

We finally obtain (3.6) by integrating the Taylor approximation of order 1 to $f^{(1)}(x)$ around $x = i/N$ and by noticing that for $z \geqslant 1 + 1/m$ and $x \in [0, 1]$, we have

$$-m^2 \leqslant f^{(2)}(x) < 0 \tag{3.7}$$

In the same way, the integration of the Taylor approximation of order 2 to $f(x)$ around $x = i/N$ with the use of (3.3) and (3.7) leads to

$$\frac{m^2}{6N} \leqslant \ln G_N\left(\frac{v}{v_0}\right) - N \cdot \int_0^1 f(x)\,dx + \frac{1}{2N} \cdot \sum_{i=0}^{N-1} f^{(1)}\left(\frac{i}{N}\right) < 0 \tag{3.8}$$

Performing the integration, the second part of the lemma follows from (3.5) and (3.6). (This proof is based on a suggestion made by the referee.)

Proof of Lemma 2. The function $Nh_c(v)$ is at least five times differentiable along $]v_0, +\infty[$ and thus has a Taylor's expansion of order 4 around v_c: if $x \in [A, B]$ then

$$Nh_c\left(\frac{x}{N^{1/4}} + v_c\right) = Nh_c + \frac{1}{4!}x^4 h_c^{(4)}(v_c) + \frac{1}{5!}N^{-1/4}x^5 h_c^{(5)}\left(v_c + \frac{x}{N^{1/4}}\right)$$

$$0 < \theta < 1 \tag{3.9}$$

since at the critical point $h_c^{(1)}(v_c) = h_c^{(2)}(v_c) = h_c^{(3)}(v_c) = 0$. From the continuity of

$$\frac{x^5}{5!} h_c^{(5)}\left(v_c + \theta \cdot \frac{x}{N^{1/4}}\right)$$

on a closed and bounded interval, we deduce that there exists x^* (respectively, y^*) where this function takes its maximal (respectively, minimal) value which we denote by z_2 (respectively z_1).

The other parts of the lemma may be proved in the same way.

Proof of Lemma 3. Let us rewrite $G_N(z)$ as

$$G_N(z) = \frac{1}{N^N}\left[N(z-1)+1\right] \cdots \left[N(z-1)+N\right] \tag{3.10}$$

Consider the following inequality[13]: for any positive real number x and an integer $n \geqslant 2$

$$n - 1 + \ln\left[(x+1)(x+2)\cdots(x+n-1)\right]$$

$$< (x+n)\ln(x+n) - (x+1)\ln(x+1) \tag{3.11}$$

With $x = N(z-1)$ and $n = N + 1$, some algebra leads to

$$\ln G_N(z) - N\left[z\ln z - (z-1)\ln(z-1)\right] < -N + 1 + \ln(N+1) \tag{3.12}$$

The result follows from (2.8) by noticing that $h_c(v)$ is decreasing along $[v_0, v_0(1+p)]$.

Proof of Lemma 4. The basis for the following proof may be found, e.g., in Ref. 14. Let us define

$$b(v) \equiv h_c(v) - h_c \tag{3.13}$$

whence, with $x = v - v_c$,

$$e^{Nh_c} \int_{v_0(1+p)}^{+\infty} e^{-Nh_c(v)} \frac{dv}{(1 - v_0/v)^{1/2}} = \int_{v_0(p-1)}^{+\infty} e^{Nb(x+v_c)} k(x)\, dx \tag{3.14}$$

where the function k is defined in (2.23) and is such that for $x \geqslant v_0(p-1)$

$$k(x) \leqslant \left(\frac{p+1}{p} \right)^{1/2} \tag{3.15}$$

It is easily shown that $b(x + v_c)$ has the following useful properties: it has an absolute maximum at $x = 0$, where $b(v_c) = 0$; $b^{(1)}(v_c) = b^{(2)}(v_c) = b^{(3)}(v_c) = 0$ and $b^{(4)}(v_c) < 0$; $b(x + v_c)$ is continuous for $x \in]-v_0, +\infty[$; and

$$-\int_{v_0(p-1)}^{+\infty} e^{b(x+v_c)} k(x)\, dx = L(p) < +\infty$$

1. The existence of the absolute maximum implies that for any $0 < \delta < v_0(1-p)$ there exists $\eta(\delta) > 0$ such that for $|x| > \delta$

$$\int_{v_0(p-1)}^{-\delta} e^{Nb(x+v_c)} k(x)\, dx + \int_{+\delta}^{+\infty} e^{Nb(x+v_c)} k(x)\, dx < L(p) e^{-(N-1)\eta(\delta)} \tag{3.16}$$

2. For any $0 < \mu < |n(v_c)|$ we can find $\delta > 0$ such that for $|x| < \delta$

$$\int_{-\delta}^{+\delta} e^{Nb(x+v_c)} k(x)\, dx \leqslant k(-\delta) \int_{-\delta}^{+\delta} e^{Nx^4[\mu + n(v_c)]}\, dx \tag{3.17}$$

and

$$k(\delta) \int_{-\delta}^{+\delta} e^{Nx^4[-\mu + n(v_c)]}\, dx \leqslant \int_{-\delta}^{+\delta} e^{Nb(x+v_c)} k(x)\, dx \tag{3.18}$$

with

$$n(v_c) = \frac{1}{4!} b^{(4)}(v_c)$$

3. We may apply inequality (3.16) to the function $e^{Nx^4[-\mu + n(v_c)]}$ so

that $\alpha(\delta, \mu) > 0$ exists such that

$$k(\delta)\int_{-\infty}^{+\infty} e^{Nx^4[-\mu+n(v_c)]}\,dx - k(\delta)\int_{-\delta}^{+\delta} e^{Nx^4[-\mu+n(v_c)]}\,dx < \frac{k(\delta)ce^{-(N-1)\alpha(\delta,\mu)}}{|n(v_c)-\mu|^{1/4}} \tag{3.19}$$

4. Adding (3.16) and (3.17) [respectively, (3.18) and (3.19)] and taking into account (3.13) we obtain (2.22b) [respectively, (2.22a)].

ACKNOWLEDGMENT

We thank the referee for helpful criticism and suggestions.

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