

# The critical region in the Percus–Yevick approximation. A numerical study for a Lennard-Jones potential

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(Received 24 June 1982; accepted 6 August 1982)

The Percus–Yevick equation is numerically solved by using the compressibility equation of state, and its behavior near the critical point is analyzed. We have used a Lennard-Jones potential without truncation, assuming an asymptotic form for the direct correlation function. The results show that the equation of state in the critical region has the same structure as the one obtained from the van der Waals equation. Then, the classical values of the critical exponents are obtained. Furthermore, the critical isotherm, the coexistence curve, and the spinodal curve are symmetrical around the critical point. Thus, the nonclassical behavior of the Percus–Yevick equation seems to be restricted to a certain class of interaction potentials.

## I. INTRODUCTION

The study of the critical behavior predicted by the approximate integral equations for classical fluids has received a great attention during the last few years. This is due to recent results seeming to indicate a nonclassical behavior in some cases and also to the desire of clarifying the relation between the approximate integral equations and the modern theories of critical phenomena. In fact, the work presented here was prompted and stimulated by some comments by Fisher and Fishman,<sup>1</sup> who showed that the available numerical results were not accurate enough to clearly decide whether the Percus–Yevick approximation provides a fully classical description of critical phenomena.

The behavior of a fluid near its critical point can be described by the critical exponents and the critical amplitudes.<sup>2,3</sup> The behavior of the pressure  $p$  along the critical isotherm  $T_c$  near the critical point  $(\rho_c, p_c)$ , is characterized by the critical exponent  $\delta$  and the critical amplitudes  $W_{\pm}$ , defined by

$$|p/p_c - 1| \approx W_{\pm} |\nu|^{\delta}; \quad \rho - \rho_c \rightarrow 0^{\pm}, \quad T = T_c, \quad (1.1)$$

where

$$\nu \equiv \rho/\rho_c - 1,$$

and  $W_+$  and  $W_-$  refer to  $\nu > 0$  and  $\nu < 0$ , respectively.

The critical exponent  $\gamma$  describes the behavior of the isothermal compressibility  $K_T$  along the critical isochore for temperatures above  $T_c$ ,

$$\hat{\chi} \approx C^+ \theta^{-\gamma}; \quad T - T_c \rightarrow 0^+, \quad \rho = \rho_c, \quad (1.2)$$

where

$$\hat{\chi} \equiv k_B T_c (\partial \rho / \partial p)_T = \rho k_B T_c K_T,$$

and

$$\theta \equiv T/T_c - 1.$$

For temperatures  $T$  below  $T_c$ , the compressibility is measured at the points characterized by the densities  $\rho_-(T)$  and  $\rho_+(T)$  on the coexistence line

$$\hat{\chi} \approx C_{\pm}^{\pm} |\theta|^{-\gamma'}; \quad T - T_c \rightarrow 0^-, \quad \rho = \rho_{\pm}(T), \quad (1.3)$$

where the amplitudes  $C_+^+$  and  $C_-^-$  correspond, respectively, to the considered limits.

The shape of the coexistence line near the critical point is given by

$$|\rho_{\pm}/\rho_c - 1| \approx B_{\pm} |\theta|^{\beta}; \quad T - T_c \rightarrow 0^-. \quad (1.4)$$

The critical exponents  $\alpha$  and  $\alpha'$  describe the behavior of the specific heat at constant volume

$$c_v \approx D_+ \theta^{-\alpha}; \quad T - T_c \rightarrow 0^+, \quad \rho = \rho_c, \quad (1.5)$$

$$c_v \approx D_- |\theta|^{-\alpha'}; \quad T - T_c \rightarrow 0^-, \quad \rho = \rho_c. \quad (1.6)$$

The van der Waals–Maxwell theory leads, for a three-dimensional fluid, to the following values of these critical exponents<sup>2</sup>:

$$\delta = 3, \quad \gamma = \gamma' = 1, \quad \beta = \frac{1}{2}, \quad \alpha = \alpha' = 0. \quad (1.7)$$

These values are usually termed in the literature as the classical values of the critical exponents. The results  $\alpha = \alpha' = 0$  indicate in this case a finite discontinuity of  $c_v$ . With respect to the critical amplitudes, the van der Waals–Maxwell theory yields

$$W_-/W_+ = C_-^-/C_+^+ = B_-/B_+ = 1, \quad C^+/C_{\pm}^{\pm} = 2. \quad (1.8)$$

These classical values greatly differ from the experimental ones<sup>3</sup> and from the values predicted by the modern theories of critical phenomena.<sup>4</sup>

On the other hand, the approximate integral equations for classical fluids give a satisfactory picture of the behavior of fluids, especially for low densities and/or high temperatures.<sup>5</sup> Nevertheless, the predictions of these integral equations in the critical region are not sufficiently known. The need of carrying out more accurate calculations than the presently existing ones has been recently pointed out by Fishman and Fisher.<sup>1,6</sup>

Near the critical point, one of the best theoretically studied integral equations is the Yvon–Born–Green (YBG) equation. This equation leads to a nonphysical, anomalous behavior for  $d \leq 4$ , where  $d$  represents the dimensionality of the system.<sup>6,7</sup> More concretely, if there existed a critical point the correlation function would take negative values near criticality at long range. Recent numerical calculations show that, for  $d=3$  and for square-well potential, this equation has no critical point.<sup>8</sup> For  $d > 4$  the YBG equation presents a purely classical behavior.<sup>7,9</sup>

In this paper, we are concerned with the Percus-Yevick (PY) equation. Baxter<sup>10</sup> solved analytically the compressibility equation of state with the PY approximation for a "sticky hard spheres" system, i. e., for a system of particles interacting via a potential of the form

$$u(r)/k_B T = \lim_{a \rightarrow 0} \begin{cases} \infty & ; r \leq \sigma, \\ \ln[12\tau a/\sigma] & ; \sigma < r \leq \sigma + a, \\ 0 & ; r \geq \sigma + a, \end{cases} \quad (1.9)$$

where  $\tau$  is a dimensionless measure of the temperature. Baxter obtained a critical point with classical values (1.7) for the critical exponents. However, this analytical solution predicts nonclassical relations<sup>1,10</sup> for the critical amplitudes:  $W_-/W_+ \approx 34$ ,  $C_-^*/C^* \approx 2$ , and  $C_-^*/C_- \approx 6.7$ . Furthermore, spinodal points (points with temperatures  $T < T_c$  such that  $\hat{\chi}^{-1} = 0$ ) exist only for  $\rho > \rho_c^-$ . Finally, the specific heat  $c_v$  logarithmically diverges on the critical isochore and when the critical isotherm is crossed at densities above critical. Fishman and Fisher<sup>1</sup> have shown that these results are related with the fact that the scaling functions are nonclassical. Obviously, the question posed now is whether this nonclassical behavior is due only to the sticky hard sphere limit or whether the PY equation has a nonuniversal critical behavior for general potentials, even if exponents are classical.

For more realistic potentials, the solution of the PY equation requires numerical methods. For a Lennard-Jones (LJ) truncated potential<sup>11</sup> and for the same potential without truncation,<sup>12</sup> the PY equation has been numerically solved and the classical values for the critical exponents have been obtained. However, a detailed study of the critical amplitudes using the solution of the PY equation has not been carried out as yet. This study is needed in order to reach a definitive conclusion about the possible nonuniversal critical behavior of the PY equation for general potentials.

The purpose of this paper is to carry out a rather detailed and complete numerical study of the behavior of a LJ fluid in the critical region described by the PY equation. The results obtained by us show a purely classical behavior for both the critical exponents and the critical amplitudes. This fact indicates that the deviation of the PY equation from the classical behavior is reduced to systems with a peculiar type of interaction potentials.

## II. NUMERICAL METHOD

The thermodynamical properties of a simple fluid in equilibrium can be obtained from the radial distribution function  $g(r)$ . In particular,

$$z \equiv p/\rho k_B T = 1 - \frac{2}{3}\pi(\rho/k_B T) \int_0^\infty dr r^3 u'(r)g(r), \quad (2.1)$$

$$\chi^{-1} \equiv (k_B T)^{-1}(\partial p/\partial \rho)_T = 1 - 4\pi\rho \int_0^\infty dr r^2 c(r), \quad (2.2)$$

$$E = \frac{3}{2}k_B T + 2\pi\rho \int_0^\infty dr r^2 u(r)g(r), \quad (2.3)$$

where  $E$  represents the internal energy per particle and  $u(r)$  is the molecular interaction potential. In Eq. (2.2),  $c(r)$  is the so-called direct correlation function, which is defined from  $g(r)$  by means of the Ornstein-Zernike relation

$$h(r) \equiv g(r) - 1 = c(r) + \rho \int d\mathbf{r}' h(r')c(|\mathbf{r} - \mathbf{r}'|). \quad (2.4)$$

Equations (2.1), (2.2), and (2.3) are usually referred to as pressure, compressibility, and energy equation of state, respectively. These equations are equivalent if one uses the exact  $g(r)$ , but this is not the case if an approximate  $g(r)$  is introduced.

In the PY approximation, the Ornstein-Zernike relation is closed by using the equation

$$c(r) = g(r)\{1 - \exp[u(r)/k_B T]\}. \quad (2.5)$$

In order to numerically solve the system of Eqs. (2.4) and (2.5), it is useful to introduce an auxiliary function smoother than  $g(r)$ . We have used  $H(r) = h(r) - c(r)$ . In this way, Eq. (2.5) becomes

$$c(r) = [H(r) + 1]\{\exp[-u(r)/k_B T] - 1\}. \quad (2.6)$$

The Ornstein-Zernike relation (2.4) can be Fourier transformed and the result is

$$\tilde{H}(k) = \rho[\tilde{c}(k)]^2/[1 - \rho\tilde{c}(k)], \quad (2.7)$$

where the Fourier transform of a function  $f(r)$  is defined by

$$\tilde{f}(k) = (4\pi/k) \int_0^\infty dr r \sin(kr)f(r). \quad (2.8)$$

In our numerical calculations the direct and inverse Fourier transforms have been performed by using Lado's algorithm<sup>13</sup>

$$\tilde{f}(k_j) = (4\pi/k_j) \sum_{i=1}^{N-1} \Delta r r_i \sin(k_j r_i) f(r_i), \quad (2.9)$$

$$f(r_i) = (2\pi^2 r_i)^{-1} \sum_{j=1}^{N-1} \Delta k k_j \sin(k_j r_i) \tilde{f}(k_j), \quad (2.10)$$

where

$$\Delta r = R/N, \quad \Delta k = \pi/R, \quad r_i = i\Delta r, \quad k_j = j\Delta k,$$

$R$  is a distance such that for  $r > R$ ,  $f(r) \approx 0$ , and  $N$  is the number of points considered in the interval  $(0, R)$ . We have taken  $R = 5\sigma$  and  $N = 200$ ,  $\sigma$  being one of the parameters of the LJ potential

$$u(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]. \quad (2.11)$$

The thermodynamical properties (2.1) and (2.2) can be numerically calculated in the form

$$z = 1 - \frac{2}{3}\pi(\rho/k_B T) \times \left[ \sum_{j=1}^N \Delta r r_j^3 u'(r_j) g(r_j) + \int_R^\infty dr r^3 u'(r) \right], \quad (2.12)$$

$$\chi^{-1} = 1 - 4\pi\rho \left[ \sum_{j=1}^N \Delta r r_j^2 c(r_j) - (k_B T)^{-1} \int_R^\infty dr r^2 u(r) \right], \quad (2.13)$$

where we have assumed the asymptotic behaviors

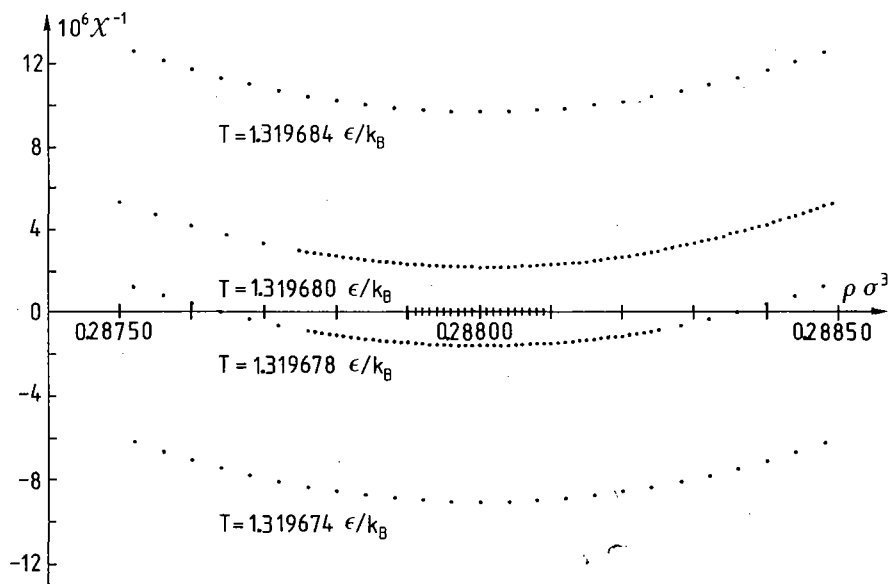


FIG. 1. Reciprocal susceptibility  $\chi^{-1} \equiv (k_B T)^{-1} (\partial p / \partial \rho)_T$  vs density for several temperatures. The critical temperature  $T_c$  has been obtained by successive interpolations and the critical density  $\rho_c$  is given by the minimum of the critical isotherm.

$$g(r) \approx 1; \quad r > R,$$

$$c(r) \approx -u(r)/k_B T; \quad r > R.$$

We have solved the PY equation by an iterative method. The input function of the  $n$ th iteration  $H_n^{in}(r)$  is introduced in Eq. (2.6) in order to obtain  $c(r)$ . Its Fourier transform  $\bar{c}(k)$ , allows us to obtain  $H(k)$  by means of Eq. (2.7) and, from its knowledge, the output function  $H_n^{out}(r)$ . Iterations are then continued in this way until the following four conditions are simultaneously satisfied:

$$\left\{ N^{-1} \sum_{j=1}^N r_j^2 [H_n^{out}(r_j) - H_n^{in}(r_j)]^2 \right\}^{1/2} < 10^{-3}, \quad (2.14)$$

$$\max_j \{ r_j |H_n^{out}(r_j) - H_n^{in}(r_j)| \} < 10^{-3}, \quad (2.15)$$

$$|1 - z_n/z_{n+1}| < 10^{-3}, \quad (2.16)$$

$$|1 - \chi_n^{-1}/\chi_{n+1}^{-1}| < 10^{-3}. \quad (2.17)$$

In the last two expressions, each subindex indicates the order of the iteration considered. These four conditions are usually redundant. Nevertheless, near the critical point, where  $\chi^{-1} \approx 0$ , condition (2.17) is more restrictive than the other ones. In fact, condition (2.17) forces the left-hand sides of Eqs. (2.14)–(2.16) to take values of the order of  $10^{-3}$ .

Henderson and Murphy<sup>11</sup> solved numerically the PY equation near the critical point for a LJ potential truncated at  $r = 6\sigma$ . The truncation of the potential allowed them to use, instead of an iterative procedure, Watts' method,<sup>14</sup> which is based on a form of the PY equation, obtained by Baxter,<sup>15</sup> valid for potentials with a finite range. In this way, Henderson and Murphy avoided assuming any asymptotic behavior for  $g(r)$ . However, this assumption has been necessary in our work because the potential we have used is not truncated. The use of Eqs. (2.1) or (2.3) would lead to significant errors because, near the critical point, the function  $g(r)$  has an infinite range. For this reason, we shall describe the

system by means of the compressibility equation of state (2.2), where only the direct correlation function, which has a finite range even near the critical point, is needed.<sup>12</sup>

### III. RESULTS

By using the numerical method described in the previous section, we have determined the direct correlation function  $c(r)$ . Inserting it into Eq. (2.2), we have obtained the results shown in Fig. 1. From these results, the following values for the critical constants are derived:

$$k_B T_c / \epsilon = 1.319679 \pm 0.000001, \quad (3.1)$$

$$\rho_c \sigma^3 = 0.28800 \pm 0.00001. \quad (3.2)$$

For the sake of consistency, it is not adequate to use the equation of state (2.1) to determine the critical pressure. We have to perform a numerical integration along the critical isotherm in Eq. (2.2). So, we have divided into 100 steps the interval of densities between  $\rho = 0$  and  $\rho = \rho_c$  and, by means of the trapezoidal rule, we have obtained

$$p_c / \rho_c k_B T_c = 0.3402 \pm 0.0003. \quad (3.3)$$

In Fig. 2 we have plotted  $\hat{\chi}^{-1}$  vs  $\theta$  for  $\rho = \rho_c$  near the critical point. We observe a linear behavior. More concretely,

$$\hat{\chi}^{-1} \approx a\theta; \quad \rho = \rho_c, \quad T - T_c, \quad (3.4)$$

where  $a \approx 2.474$ . Comparison of this result with Eq. (1.2) allows us to write that  $C^* = 1/a$  and that the critical exponent  $\gamma$  takes the classical value, i. e.,  $\gamma = 1$ . The negative values of  $\hat{\chi}^{-1}$  for  $T < T_c$  correspond to unphysical solutions. This situation is similar to the one appearing in the van der Waals equation.

The linear behavior [Eq. (3.4)] is more clearly observed in Fig. 3, where we have plotted  $\theta \hat{\chi}$  vs  $\theta$  for  $\rho = \rho_c$ . In this figure the range of temperatures considered is much greater than the one considered in Fig. 2.

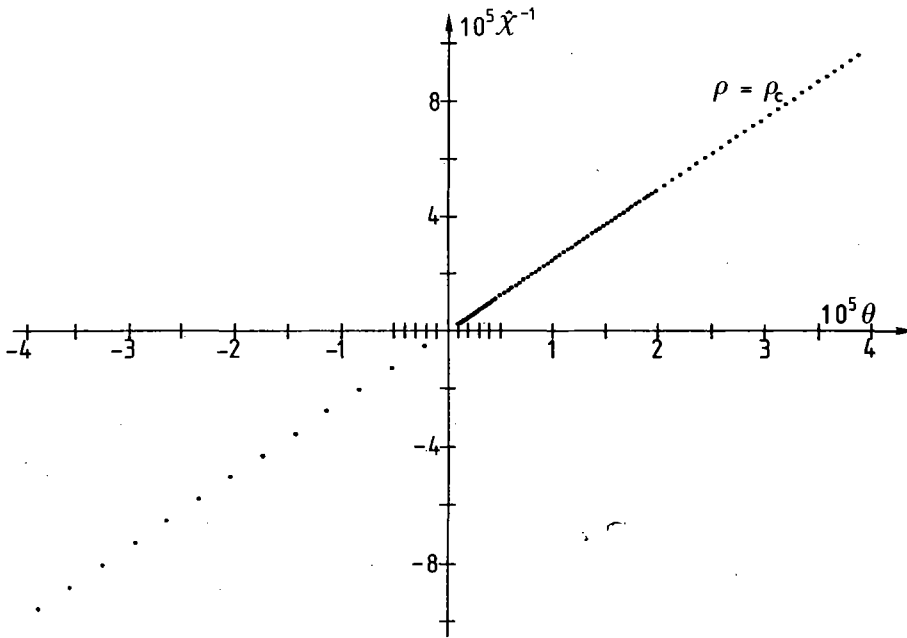


FIG. 2. Dependence of  $\hat{\chi}^{-1} \equiv (k_B T_c)^{-1} (\partial p / \partial \rho)_T$  on  $\theta \equiv T/T_c - 1$  along the critical isochore for temperatures very close to the critical one.

A representation, similar to the one of Fig. 3, but for the temperature range of Fig. 2, would show a large deviation from the linear behavior in the neighborhood of  $\theta = 0$ . This is due to the influence of the uncertainty in the determination of the critical temperature. A detailed discussion of a similar situation can be found in Ref. 16.

In Fig. 4 we have again plotted  $\theta \hat{\chi}$  vs  $\theta$  for  $\rho = \rho_c$ , but now the range of  $\theta$  has been greatly enlarged. We see that the linear behavior given by Eq. (3.4) is maintained even for temperatures far from the critical one. This is also a property of the van der Waals equation, for which  $a = 9/4$ .

In order to show simultaneously the dependence of  $\hat{\chi}$

on the density and the temperature in the neighborhood of the critical point, we have plotted  $\hat{\chi}^{-1}$  vs  $\nu^2$  for several temperatures near the critical one in Fig. 5. On the right-hand side of the figure, we have plotted points corresponding to  $\rho > \rho_c$  and on the left-hand side points corresponding to  $\rho < \rho_c$ . We observe that the isotherms are symmetrical with respect to the critical isochore ( $\nu = 0$ ) and that the points corresponding to each temperature fit accurately to straight lines of constant slope, for  $T > T_c$  as well as for  $T < T_c$ . Taking into account these results and Eq. (3.4), we can describe the asymptotic behavior of  $\hat{\chi}^{-1}$  by the equation

$$\hat{\chi}^{-1} \approx b\nu^2 + a\theta; \quad \rho \rightarrow \rho_c, \quad T \rightarrow T_c, \quad (3.5)$$

where  $b \approx 1.019$ . Setting  $\theta = 0$  in this equation and com-

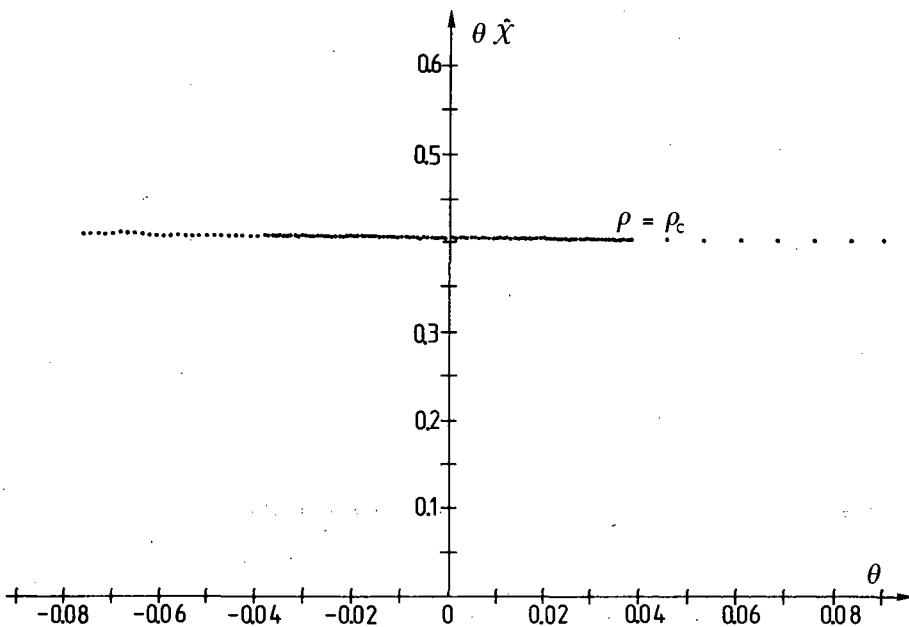


FIG. 3. Plot of  $\theta \hat{\chi}$  vs  $\theta$  along the critical isochore for temperatures close to  $T_c$ .

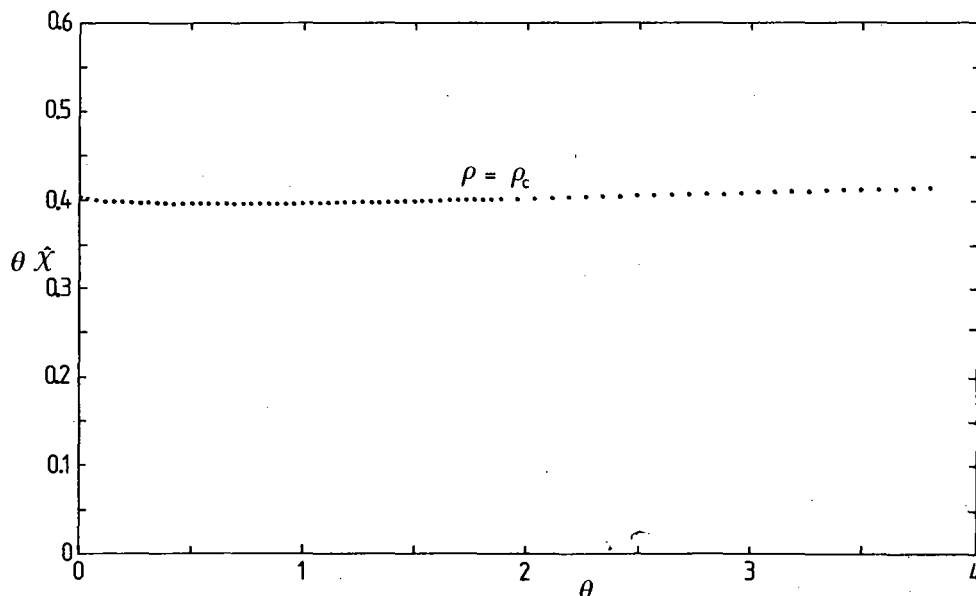


FIG. 4.  $\theta \hat{\chi}$  vs  $\theta$  along the critical isochore for a wide range of temperatures above  $T_c$ .

paring with the one obtained by taking the derivative of Eq. (2.1) with respect to  $\rho$ , we deduce that  $\delta=3$  and that  $W_+ = W_- = W = (b/3)(\rho_c k_B T_c / p_c)$ . For the van der Waals equation, a similar result can be obtained with  $b = 27/16$ .

The linear dependence of  $\hat{\chi}^{-1}$  with respect to  $\theta$  can also be obtained, without turning to Eq. (3.4), by simply studying the temperature dependence of the ordinates at the origin of the straight lines in Fig. 5. In addition, we can obtain by interpolation a value for  $T_c$  more accurate than the one given by Eq. (3.1). More concretely, we have obtained  $k_B T_c / \epsilon \approx 1.3196788$ . Nevertheless, the value (3.1) is accurate enough to be used in our calculations.

We want to emphasize that the PY equation predicts the asymptotic behavior (3.5) for  $T < T_c$  as well as for

$T > T_c$ . However, for each temperature  $T < T_c$  there exists an interval of densities corresponding to negative, unphysical values of the isothermal compressibility. This interval of densities is bounded by the values  $\rho_s^-(T)$  and  $\rho_s^+(T)$ , defining the spinodal line, at which the isothermal compressibility diverges. Taking into account the asymptotic behavior (3.5), the spinodal line near the critical point is defined by the equation

$$\nu_s^{\pm} \equiv \rho_s^{\pm} / \rho_c - 1 \approx \pm (a/b)^{1/2} (-\theta)^{1/2}; \quad \theta \rightarrow 0^- \quad (3.6)$$

From the expression (3.5), one can only obtain a partial information about the behavior of the pressure near the critical point. In order to complete this information, we have studied the temperature dependence of the pressure for  $\rho = \rho_c$ . The values of the pressure have been obtained, for each temperature, by numerically integrating  $(\partial p / \partial \rho)_T$  by means of the trapezoidal rule

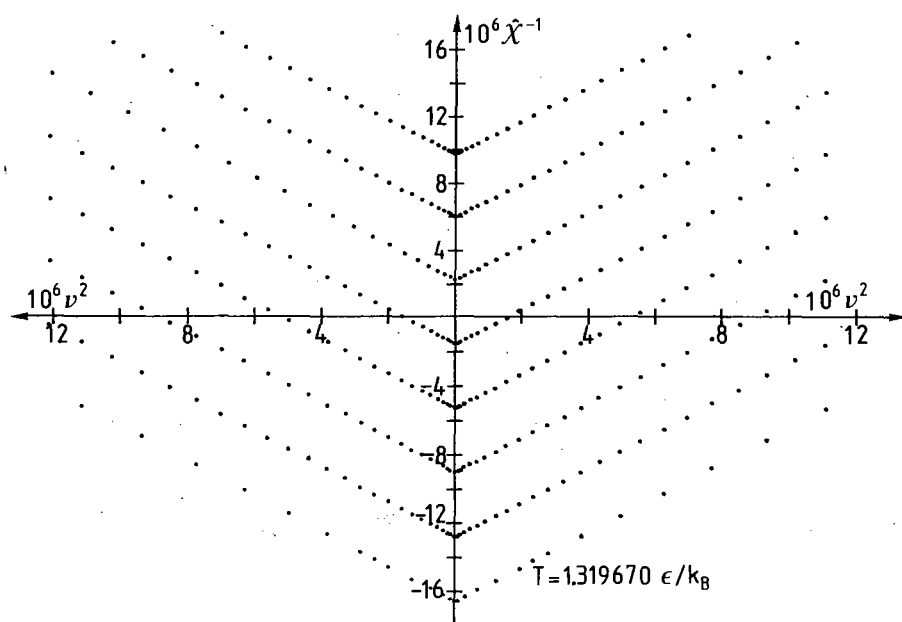


FIG. 5. Dependence of  $\hat{\chi}^{-1}$  on  $\nu^2 \equiv (\rho/\rho_c - 1)^2$  for several temperatures close to the critical one. The lowest isotherm corresponds to  $T = 1.319670 \epsilon/k_B$ . The difference between the temperatures of two successive isotherms is  $\Delta T = 2 \times 10^{-6} \epsilon/k_B$ , so the highest represented isotherm corresponds to  $T = 1.319684 \epsilon/k_B$ .

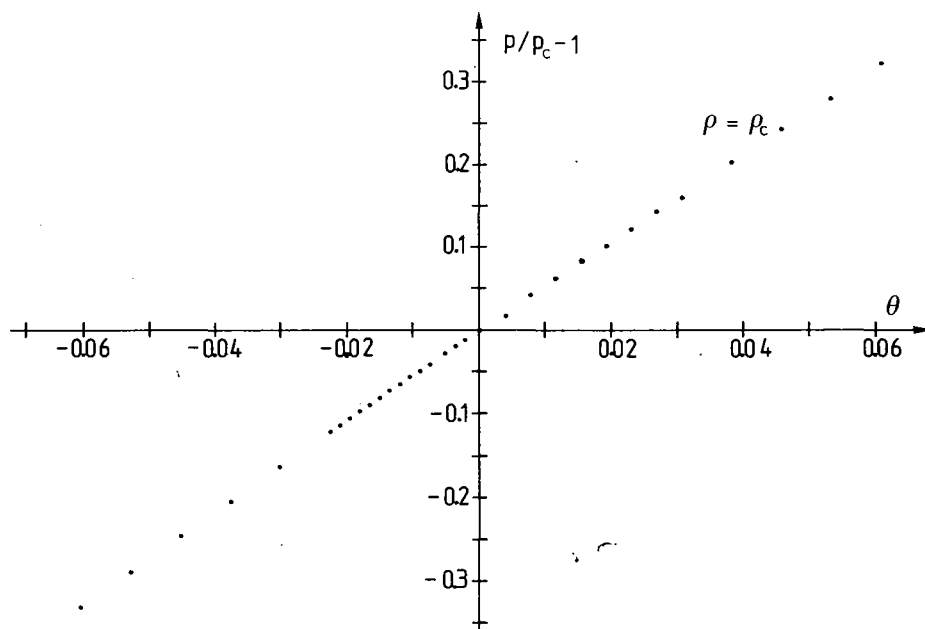


FIG. 6. Plot of  $p/p_c - 1$  vs  $\theta$  along the critical isochore for temperatures close to  $T_c$ .

and dividing the interval of densities between 0 and  $\rho_c$  into 100 steps. In Fig. 6, we have plotted  $p/p_c - 1$  vs  $\theta$  near the critical point for  $\rho = \rho_c$ . The points fit accurately to a straight line, which allows us to write the asymptotic law

$$p/p_c - 1 \approx m(T/T_c - 1), \quad T \rightarrow T_c, \quad \rho = \rho_c, \quad (3.7)$$

where  $m \approx 5.38$ . This behavior is maintained even for temperatures far above the critical one, as can be observed in Fig. 7. This linear behavior, with  $m = 4$ , is also obtained from the van der Waals equation, being valid for all temperatures. Of course, it would be interesting to establish whether the linear behavior described by Eqs. (3.4) and (3.7) can be analytically derived from the PY approximation, even when the temperature of the system is far from the critical one.

Integration of Eq. (3.5), taking into account Eq. (3.7), yields

$$p/p_c - 1 \approx Wv^3 + a'v\theta + m\theta; \quad \rho \rightarrow \rho_c, \quad T \rightarrow T_c, \quad (3.8)$$

where  $a' \equiv a(\rho_c k_B T_c / p_c)$ . This expression is the equation of state for a Lennard-Jones fluid in the critical region, obtained from the compressibility equation in the PY approximation. The van der Waals equation of state possesses the same asymptotic law, although with different numerical values for the critical amplitudes. For subcritical temperatures there exists an unphysical region for which the equation of state (3.8) gives rise to negative values for the compressibility. Making use of the Maxwell construction we can obtain the limit densities of the coexistence curve  $\rho_{\pm}(T)$

$$\nu_{\pm} \equiv \rho_{\pm} / \rho_c - 1 \approx \pm (3a/b)^{1/2} (-\theta)^{1/2}; \quad \theta \rightarrow 0^-. \quad (3.9)$$

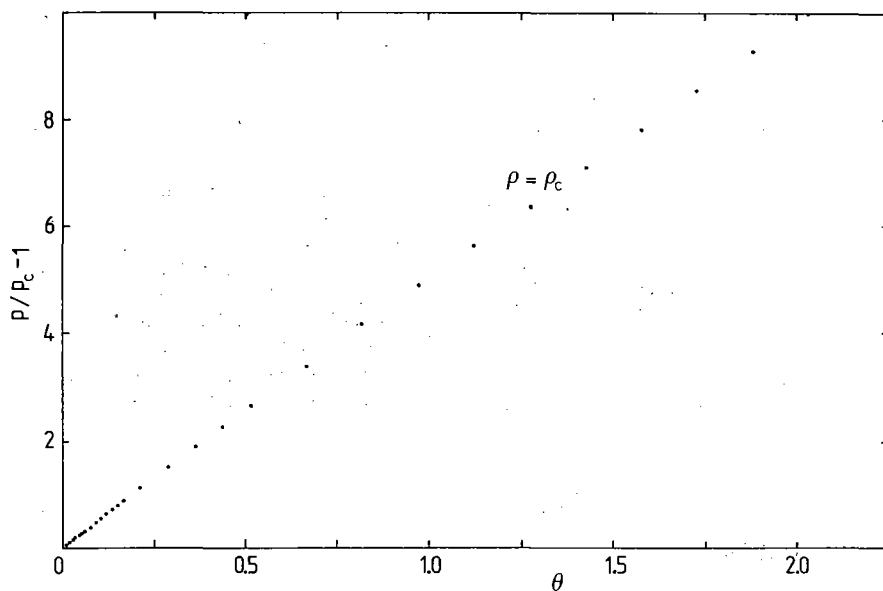


FIG. 7. Plot of  $p/p_c - 1$  vs  $\theta$  along the critical isochore for a wide range of temperatures above  $T_c$ .

Also, the vapor pressure takes the asymptotic form

$$p_v/p_c - 1 \approx m\theta; \quad \theta \rightarrow 0^- \quad (3.10)$$

Expression (3.9) shows that the critical exponent  $\beta$  takes the value  $\frac{1}{2}$  and that  $B_+ = B_- = (3a/b)^{1/2}$ . By inserting Eq. (3.9) into Eq. (3.5), we obtain

$$\hat{\chi}^{-1} \approx 2a(-\theta); \quad \theta \rightarrow 0^-; \quad \rho = \rho_c(T) \quad (3.11)$$

Comparing with Eq. (1.3), we obtain the value  $\gamma' = 1$  and the relations  $C_- = C_+ = C^*/2$ .

Finally, we are going to study the behavior of  $c_v$  near the critical point. This quantity is related to the free energy per particle  $F$  through the well-known relation

$$c_v = -T(\partial^2 F / \partial T^2)_p \quad (3.12)$$

The free energy can be obtained from the equation of state by means of the relation

$$p = \rho^2(\partial F / \partial \rho)_T \quad (3.13)$$

where our equation of state is Eq. (3.8) corrected with the Maxwell construction. To obtain  $F$ , we integrate Eq. (3.13) starting from a reference density  $\rho_0 \lesssim \rho_c(T)$  for values of  $T$  close enough to  $T_c$ . If we admit that  $F(\rho_0, T)$  is a continuous function of  $T$  we obtain

$$c_v(\rho_c, T) - c_v(\rho_0, T) \approx \begin{cases} 0 & ; T - T_c \rightarrow 0^+ \\ \frac{3}{2} k_B a^2 / b & ; T - T_c \rightarrow 0^- \end{cases} \quad (3.14)$$

This result shows that the compressibility equation of state in the PY approximation predicts a finite discontinuity of the specific heat  $c_v$ . Then, the critical exponents  $\alpha$  and  $\alpha'$  take the classical value 0.

#### IV. SUMMARY

We have shown that the PY approximation with a LJ potential gives a purely classical behavior. The main result of this paper is Eq. (3.8), which is formally equivalent to the one that could be obtained from the van der Waals equation.

We want to emphasize the internal consistency of our method in the sense that we have only used the compressibility equation of state (2.2). Henderson and Murphy<sup>11</sup> obtained the values of the critical exponents

$\alpha$  and  $\beta$  by means of the energy equation of state (2.3). Their reason for using Eq. (2.3) was the great difficulty involved in the numerical solution of Eqs. (3.12) and (3.13), that would lead to significant errors. Our numerical results allows us to write the equation of state near the critical point and, from it, the critical exponents  $\alpha$  and  $\beta$  can then be obtained by simple analytical calculations.

#### ACKNOWLEDGMENTS

We are grateful to Professor M. E. Fisher for his valuable suggestions and comments about the questions treated in this paper. This work has been supported in part by the Spanish Government through the Comisión Asesora Científica y Técnica.

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