Construction of an effective Hamiltonian for a three-dimensional Ising universality class

A. Brognara,[1,3] A. Parola,[2,3] and L. Reatto[1,3]
[1]*Università di Milano, Via Celoria 16, 20133 Milano, Italy*
[2]*Dipartimento di Fisica, Università dell'Insubria, Via Lucini 3, Como, Italy*
[3]*Istituto Nazionale per la Fisica della Materia, Milano, Italy*
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The asymptotic and preasymptotic critical behavior in fluids, mixtures, and uniaxial magnets is believed to be described by an effective φ^4 scalar field theory with suitable, nonuniversal, coupling constants. The critical parameters as well as the extent of crossovers and corrections to the leading critical behavior in physical systems, crucially depends on the choice of these couplings. Here we propose a new method for deriving the effective scalar field theory appropriate to a microscopic model in this universality class. Use is made of the hierarchical reference theory, which implements the basic ideas of Wilson momentum space renormalization group to microscopic Hamiltonians. The effective low-energy field theory is then analyzed by the minimal subtraction scheme of Schloms and Dohm. We discuss the application of this method to the three-dimensional Ising model and to the liquid-vapor phase transition. We make comparison with high-temperature expansion results and with experimental data for rare gas.

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I. INTRODUCTION

Following the universality paradigm, physical systems presenting phase transitions are grouped in universality classes according to their asymptotic critical behavior. Of particular physical relevance is the three-dimensional (3D) Ising universality class, which includes easy axis magnets, fluids, and mixtures.

Nowadays it is well known that, in the critical region, all these systems are described by a φ^4 scalar field Hamiltonian H_{eff} [1] which physically describes the long-wavelength fluctuations of the order parameter. This effective Hamiltonian depends on two coupling constants: the bare mass r and the self-interaction u of the field. Although the universal quantities (i.e., critical exponent and amplitude ratios) are independent of the value of $u>0$, this is not so for many physically interesting properties in the asymptotic and preasymptotic. For instance, the critical temperature, the amplitude of order parameter fluctuations, the extension of the critical region, the importance of corrections to scaling, the presence of detectable crossover regions with well-defined effective critical exponents, all depend on the particular value of the self-interaction term in H_{eff} which governs the coupling of fluctuations on different lengthscales.

Actually, some doubt on the accuracy of a φ^4 effective Hamiltonian for describing the preasymptotic critical behavior of the Ising model has been reported in the literature [2]. In particular, the possible relevance of higher-order interactions (like a φ^6 term) or of irrelevant symmetry breaking terms (such as φ^5) should be investigated.

Quite accurate nenormalization-group (RG) methods have been developed for obtaining the physically relevant quantities out of a φ^4 effective Hamiltonian [3–6]. Using either large order ϵ-expansion results near dimension four or weak-coupling expansion of the β function in a Callan-Symanzik equation, explicit expressions for the order parameter, correlation length, and susceptibility of the φ^4 model can be evaluated. The missing ingredient is still the link between a specific microscopic model and the effective coarse grained Hamiltonian, which requires the tracing out of all ''short-wavelength'' fluctuations.

In order to clarify these issues, it is therefore important to find a systematic way to build up an effective Hamiltonian out of a given microscopic model. The natural tool to address this class of problems is the hierarchical reference theory of fluids (HRT) [7,8] which implements the basic ideas of Wilson momentum space RG in the framework of liquid state theory.

This theory allows, starting from the microscopic Hamiltonian of the model, to derive an exact hierarchy of differential equations describing the evolution of the n-point correlation function of the system when fluctuations on larger and larger lengthscales are included.

However, in order to go beyond dimensionality expansion, it is necessary to introduce some kind of approximation into the theory (closure or truncation).

In the numerical analisys of HRT performed so far, only the first equation of the hierarchy has been treated by imposing an Ornstein-Zernike (OZ) form for the pair-correlation function. The results obtained are in good agreement with experiments and simulations, satisfying scaling and hyperscaling with nonclassical critical exponents whose values, however, typically deviate from the exact ones by 5%–10%. The description of first-order phase transitions should also be improved because HRT predicts an unphysical divergence of the compressibility at coexistence.

It is important to point out that these problems are only due to the introduction of an approximate closure relation and do not represent a limitation of HRT. In fact, it has been verified [8] that the second-order ϵ expansion of the hierarchy correctly reproduces the well-known results obtained by Wilson [1] for the critical exponents.

The good accuracy of HRT on the description of the fluid in regions not asymptotically close to a phase transition, suggests that the key ingredient missing in HRT with the present closure is just the correct treatment of very long-wavelength fluctuations, which determine the universal quantities. On the other hand, we know that, on those lengthscales, the model is well represented by a coarse grained effective Hamiltonian, possibly of the φ^4 form. Therefore, it is rather natural to attempt to use the HRT formalism to trace out fluctuations up to a certain wave vector cutoff Λ, and then switch to a field theoretical description based on an effective Hamiltonian. This is precisely the program of this paper, which will be presented in the following sections.

Section II contains a brief summary of the HRT formalism, to make the paper self-contained, together with the discussion of the method we used to extract from HRT the couplings of the effective Hamiltonian. The RG equation we adopted to analyze the effective Hamiltonian, is also reported. In Sec. III we show three applications of this formalism to the Ising model and to two models of fluids. Section IV contains some conclusion and perspective.

II. THEORY

A. HRT equations

Let us consider the equilibrium properties of a classical fluid consisting of particles interacting through the two-body potential $v(r)$. The starting point in the derivation of HRT equations is the separation of the interatomic interaction $v(r)$ in two parts [8]:

$$v(r)=v_R(r)+w(r). \tag{1}$$

Here $v_R(r)$ is a short-range (mostly) repulsive term (reference) whose thermodynamic and structural properties are assumed known, at least numerically. Instead, $w(r)$ is an attractive term, which triggers the phase transition. Using this separation and performing a Legendre transformation on the grand canonical partition function, a formal diagrammatic expansion for the Helmoltz free energy can be written at all orders in perturbation theory. In order to describe the evolution of the thermodynamic quantities due to the inclusion of fluctuations, we implement the basic ideas of Wilson's RG approach [1] within such a formal perturbative expansion. We first define a sequence of intermediate "attractive" potentials characterized by an infrared cutoff Q in Fourier space:

$$w^Q(k)=\begin{cases} w(k), & k>Q \\ 0, & k<Q, \end{cases} \tag{2}$$

and we study how the properties of the system, interacting via $v^Q(r)=v_R(r)+w^Q(r)$, evolve when Q is varied form ∞ down to 0. In this way, the Fourier components of the attractive part of the physical interaction may be included selectively, starting form the shorter wavelengths; in fact in the $Q\to\infty$ limit $w^Q(k)$ vanishes and we reduce to the reference system, while as $Q\to 0$ the full interaction $v(r)$ is recovered. Physically, this procedure corresponds to inhibit fluctuations over wave vectors smaller than Q, thereby reproducing the momentum shell integration RG. At level Q, effects due to the nonlinear coupling of density fluctuations are retained only for $k>Q$; we will refer to such a system as the Q system. Notice that with this approach, no operation of coarse graining is performed and all length scales are present in the Q system. The special choice (2) for the interatomic interaction is able to allow the gradual turning on the long-wavelength fluctuations typical of RG.

Remarkably, it is possible to obtain an exact set of differential equations expressing the change in physical properties when the cutoff Q is varied. They have the structure of a hierarchy of evolution equations for the free energy and the n-point correlation functions. Here we only report the first equation of the hierarchy, which governs the inclusion of fluctuations in the Helmholtz free energy of the model

$$-\frac{d}{dQ}\left(\frac{-\beta\mathcal{A}^Q}{V}\right)=\frac{1}{2}\int_{k=Q}\frac{d\Omega_k}{(2\pi)^3}\ln[1+\rho\mathcal{S}^Q(k)\phi(k)], \tag{3}$$

where $\phi=-\beta w$, while $\mathcal{A}^Q/V$ and $\mathcal{S}^Q(k)$ are, respectively, the free-energy density and the structure factor of the Q system. At the beginning of the integration ($Q\to\infty$) both these quantities acquire their mean-field values, which in fact neglect the nonlinear coupling of fluctuations.

The second equation of the hierarchy relates the Q derivatives of $\mathcal{C}^Q(k)$ to the three- and four-point correlation functions. Analogously the other equations of the hierarchy give relations that link the Q derivative of the n-point correlation function to the correlation functions of order up to $n+2$. This formal hierarchy of equations is exact in the whole phase diagram of the model. However, in order to obtain a closed-form equation, which can be numerically solved, we must introduce some approximation. We will consider the first equation of the hierarchy with a closure relation expressing the structure factor $\mathcal{S}^Q(k)$ in terms of the free energy $\mathcal{A}^Q$. This closure is inspired by the so-called optimized random phase approximation of liquid state theory, which is known to describe the structure of a fluid rather accurately [9]. The details of this closure can be found in Ref. [8]. Here we only point out that this approximation belongs to the class of the "Ornstein-Zernike" closures characterized by the analyticity of the correlation function in a neighborhood of $k=0$, even at the critical point:

$$\frac{1}{\rho\mathcal{S}^Q(k)}\overset{k\to 0}{\sim}-\frac{\partial\mathcal{A}^Q}{\partial\rho^2}+b_0k^2, \tag{4}$$

where b_0 is a nonuniversal constant, related to the microscopic interaction and assumed to be finite in the whole phase diagram of the model. At $k=0$, this relation is exact and gives the compressibility sum rule. Closure relation (4) unavoidably implies the vanishing of the critical exponent η, thereby introducing serious approximations in the evaluation of universal properties at the critical point.

The growth of the long-wavelength fluctuations in the critical region makes this relation (4) less and less accurate as Q goes to zero, leading to a not very accurate determination of the critical exponents and to an unphysical divergence of the compressibility when the coexistence curve is approached.

In Sec. III A we will discuss an application to the Ising model on a square lattice. Treatment of lattice systems require some modification to HRT equations presented above (details can be found in Refs. [8,10]). Here we only recall that the integration in real space is replaced by sums, and momentum space integration must be limited to the first Brillouin zone. Due to the anisotropy of the boundary of this zone, integration over the spherical surface $|\boldsymbol{k}|=Q$ in Eq. (3) is not appropriate, but the integration can be performed over any surface Σ_Q that spans the Brillouin first zone. The particular form of the potential and of the closure relation make the following choice for the surface very convenient:

$$\Sigma_Q=\left\{\boldsymbol{k}: \frac{1}{2}-\frac{1}{2d}\sum_{\alpha=1}^{d}\cos k_\alpha=Q\right\}. \tag{5}$$

B. The critical region in the HRT

If the system is in the critical region and we analyze the asymptotic evolution at long wavelengths (i.e., as $Q\rightarrow 0$) Eq. (3) with the low k form of the closure relation (4) can be written in a universal form, independent of the details of the microscopic interaction:

$$l\frac{\partial H^Q}{\partial l}+\frac{1}{2}z\frac{\partial H^Q}{\partial z}-dH^Q=\frac{1}{2}\ln\left(\frac{1+\partial^2 H^Q/\partial z^2}{1+(\partial^2 H^Q/\partial z^2)|_{z=0}}\right). \tag{6}$$

Here the following definitions have been employed:

$$H^Q=-\frac{1}{K_d}Q^{-d}\left(\frac{-\beta\mathcal{A}^Q}{V}-\frac{-\beta\mathcal{A}^Q}{V}\bigg|_{\rho=\rho_0}\right), \tag{7}$$

$$z=\left(\frac{b_0}{K_d}\right)^{1/2}(\rho-\rho_0)Q^{-(d-2)/2}, \tag{8}$$

where for $d=3$, $K_d=(2\pi^2)^{-1}$, and $Q=Q_0/l$, ρ_0 is the critical density and the initial condition is set at $Q=Q_0$. Equation (6), with some straightforward substitution [8,11], is formally identical to a Wegner-Hougton RG equation for a scalar field theory in the local potential approximation (LPA) [12]. This equation describes the RG flow of an effective Hamiltonian of the type

$$H_{eff}=\int\left[\frac{1}{2}(\boldsymbol{\nabla}\varphi(x))^2+v_2\varphi^2(x)+\sum_{m=3}^{\infty}v_m\varphi^m(x)\right]d^dx \tag{9}$$

as fluctuations are included under the assumption that the RG flow does not generate nonlocal effective interactions. This is in fact an approximation, similar in spirit to our OZ closure (4). In Eq. (9) the ultraviolet (UV) cutoff $|q|<1$ on the momentum of the Fourier transformed fluctuating field φ_q, is also understood. The identity between the asymptotic form of the HRT equation and the RG equations for a scalar field in LPA, allows us to identify, in the long-wavelength regime, the expansion coefficients r_0 of the local potential V in the effective Hamiltonian (9) with the derivatives of the HRT free energy evaluated at Q_0:

$$v_m=\frac{1}{(m)!}\frac{Q^{m/2-3}}{b^{m/2}}\frac{\partial^m}{\partial\rho^m}\left(\frac{\beta\mathcal{A}^Q(\rho)}{V}\right)_{\rho=\rho_c}\Bigg|_{Q=Q_0}. \tag{10}$$

The integration over the short-wavelength fluctuations ($Q>Q_0$), performed by the HRT evolution equations, together with the defining relation (10) allows us to connect the microscopic model interacting via the potential (1) with an effective Hamiltonian of the form (9) which describes the long-wavelength effective model appropriate to our physical system. Within this scheme, all the short-wavelength details of the microscopic model are explicitly integrated out and contribute to the definition of the expansion coefficients (self-interactions) in the effective Hamiltonian. These values are therefore specific to the particular model we are studying. Conversely, universal quantities like critical exponents and amplitude ratios are the same for all models of the 3D Ising universality class. The effective Hamiltonian constructed by this method describes the long-wavelength fluctuations of the system in the momentum range from Q_0 to 0, which drive the critical behavior. However, it also retains the information about the nonuniversal properties of the system through the values of the interactions v_m, which do depend on the microscopic structure of the model.

C. Dohm equations

At this stage we have just developed a systematic way to derive an effective Hamiltonian describing the physical system in the critical region. In order to obtain the physical properties of the microscopic model we have to resort to some method able to calculate averages and correlation functions for field theoretical Hamiltonians of this form. This Hamiltonian represents a self-interacting real scalar field and is supplemented by an UV cutoff Λ. This program can be efficiently achieved in the context of minimal subtraction RG scheme [13]. In particular, we choose the formulation due to Schloms and Dohm [3,4], where renormalization is performed directly in three dimensions without using the ϵ-expansion technique. Furthermore, Dohm already gives expressions for various physical observables above and below the critical temperature, and the renormalizing functions employed are known from accurate Borel resummation of high loop order perturbative expansion. This allows us to obtain very accurate results for universal quantities whose values are reported in Refs. [3,4,14]. This method has been applied just to a φ^4 theory, and therefore we assume to truncate our general local potential $V(\varphi)$ in Eq. (9) to fourth order. We only recall the main steps in deriving these RG equations. The starting point is therefore the bare Hamiltonian for a φ^4 theory:

$$H_\varphi=\int d^dx\left[\frac{1}{2}r_0\varphi_0^2+\frac{1}{2}(\boldsymbol{\nabla}\varphi_0)^2+u_0\varphi_0^4\right]. \tag{11}$$

In Eq. (11) the odd powers have been neglected because, close to the transition, the effective Hamiltonian is invariant under the change $\varphi \to -\varphi$, and higher-order powers are irrelevant in the RG sense.

The expressions for the susceptibility and correlation length are

$$\mathring{\chi}(k) = \mathring{\Gamma}^{(2)}(k, r_0, u_0, \Lambda, d)^{-1}, \tag{12}$$

$$\xi(r_0, u_0, \Lambda, d) = \{\mathring{\chi}(0)[\mathring{\chi}(k)^{-1}]|_{k=0}\}^{1/2}, \tag{13}$$

where $\mathring{\Gamma}^{(N)}$ are the bare vertex functions. The critical value of r_0 (r_{0c}) is implicitly defined by

$$\mathring{\Gamma}^{(2)}(0, r_{0c}, u_0, \Lambda, d) = 0. \tag{14}$$

This allows us to express the vertex functions in terms of the difference $r_0 - r_{0c}$, which will be convenient by virtue of the super-renormalizability of a φ^4 theory below four dimensions. The theory is then regularized at a certain value of the momenta (subtraction point) using the minimal subtraction scheme [13]. Finally, the use of Callan-Symanzik equations, allows us to obtain finite renormalized vertex functions, expressed in terms of renormalized quantities, at every energy. Integration of the Callan-Symanzik equation leads to the following expression for the susceptibility:

$$\chi = \mathring{\chi}(k=0) = Z_\varphi(u) f^{(2)}[1, u(l), 3]^{-1} l^{-2} \exp \int_{u(l)}^{u} \frac{\zeta_\varphi(u')}{\beta_u(u')} du', \tag{15}$$

$$\frac{du(l)}{d \ln l} = \beta_u[u(l), 1] \quad \text{with} \quad u(l=1) = u = Z_u^{-1} Z_\varphi^2 K_3 u_0. \tag{16}$$

Here $1 < l < \infty$ is the renormalization parameter (measured in mass units of $1/\mu$) which defines the momentum scale of the renormalization point. The functions $\zeta_\varphi(u)$, $Q(1,u,3)$, $\zeta_r(u)$, $\beta_u(u)$, and $Z_r(u)$ are known by Borel summation of perturbative loop expansion [3,4,14]. Now, using the expansion coefficients (10) as initial conditions for the Dohm equations, we are able to obtain the behavior of quantities of physical interest.

The above procedure can also be performed below T_c. We only report the Dohm equations for susceptibility and order parameter [4]:

$$\chi_-(k) = Z_\varphi(u) f_-^{(2)}[u(l_-)]^{-1} l_-^{-2} \exp \int_{u(l_-)}^{u} \frac{\zeta_\varphi(u')}{\beta_u(u')} du', \tag{17}$$

$$\langle \varphi_0 \rangle^2 = Z_\varphi(u) f_\varphi[u(l_-)] l_- \exp \int_{u(l_-)}^{u} \frac{\zeta_\varphi(u')}{\beta_u(u')} du', \tag{18}$$

$$\frac{du(l_-)}{d \ln l_-} = \beta_u[u(l_-), 1] \quad \text{with} \quad u(l_- = 1) = u = Z_u^{-1} Z_\varphi^2 K_3 u_0. \tag{19}$$

In this case, however, the renormalizing functions for the order parameter $\{Z_\varphi(u), f_\varphi[u(l)], \zeta_\varphi(u)\}$ are known with lower accuracy, so we expect a lower accuracy in the determination of this quantity.

Integration of the Dohm equations can be easily performed numerically by a standard adaptive Runge-Kutta alghoritm [15]. The only quantity, which is not given, is the value of r_{0c}; we have chosen the value obtained from the integration of HRT at the HRT critical temperature via Eq. (10). In this way, the critical temperature of the model is fixed to its HRT estimate, which is actually quite accurate in all the models we are going to examine. Another point to be discussed is that Eqs. (16) and (19) do not contain the temperature variable that just enters through the initial values of the coupling constants r_0, u_0. Even if the hypothesis of linear dependence of r on t is the most popular choice in the literature, in our case we prefer to relax this ansatz by integrating the HRT equations at every temperature of interest determining the values of r_0 and u_0 via Eq. (10). The value of l, at which we stop the integration of the Dohm equations, is implicitly defined by

$$r_0 - r_{0c} = Z_r(u,1) Q[1, u(l), 3] \exp \int_1^l (2 - \zeta_r) \frac{dl'}{l'} \tag{20}$$

and physically corresponds to the inverse correlation length

$$\xi = l^{-1}. \tag{21}$$

In summary, our method consists of integrating the HRT equations at every temperature down to a suitable value of the cutoff wave vector Q_0 in order to generate the expansion coefficients of the effective Hamiltonian. At this point, instead of proceeding with the full integration of HRT down to $Q=0$, we use the coefficients $r_0 = v_2 - v_{2c}$ and $u_0 = v_4$ obtained in this way to integrate the Dohm equations. In particular, the value of u_0 gives the initial condition, while the value of $r_0 = v_2 - v_{2c}$ is used in Eq. (20) to obtain the value of l at which we stop the integration.

III. RESULTS

Before showing the results obtained by the method discussed in the previous sections, we briefly discuss a few open questions, which are still present at this point. First of all, we have established a connection between HRT in OZ closure and Dohm equations, but we do not know what is the range of numerical values of the cutoff Q at which this identification is correct, or if such a range of values exists. In fact, as we proceed in the integration of the HRT equations, the OZ closure becomes less and less accurate, while the identification with a φ^4 theory becomes more accurate because we are entering the critical region and all irrelevant terms disappear in the effective Hamiltonian [16]. Second, if such a range of values exists, consistency requires that physical quantities must show very little dependence on the choice of the matching point in the range.

In the following discussion, all physical quantities presented are expressed in natural units, taking as unit length the lattice spacing for the Ising model and of the particle diameter σ for the fluid represented by either a Lennard-Jones (LJ) or an Aziz potential.

A. Ising model

As a first check of our method, we have considered the Ising model. Studying this model (whose properties are known with high accuracy from other methods like series expansion [17,18]) will allow us to test the proposed method to construct the effective Hamiltonian and to get some information about the matching value of the cutoff Q. In Fig. 1, we show the behavior of the first few even coefficients v_2, v_4, and v_6 as the integration of the HRT equations is carried out. The divergence of the coefficients v_2 and v_4 at $Q=0$ is due to the presence of negative powers of the cutoff in the definition (10). We only note that the divergence change from $+\infty$ to $-\infty$ is above or below the critical temperature. Looking at Fig. 1, it can be seen that the coefficient v_6 has a minimum, so one can think to fix the matching point at this value of Q, in order to minimize the effects induced by neglecting this term. In fact some authors argued that v_6 may be important in the description of the preasymptotic region [2]. Nonetheless we empirically find that the results obtained for physical quantities shows very little dependence from the matching value in the region $0.5<Q<1.25$. So we arbitrarily choose to fix at each temperature the matching value at $Q=1.0$, in order to obtain a unified criterium even for other models which do not display the minimum in the v_6 coefficient (see Fig. 4 and 8).

In Figs. 2 and 3 the reduced temperature dependence of the susceptibility, correlation length, and order parameter are shown on a decimal logarithmic plot. In this way the asymptotic slope of each quantity is identified with the relative critical exponent. Notice that the present theoretical results contain no free parameters and the comparison is performed at the same reduced temperature. We recall that the HRT critical temperature is within 0.5% from the correct value [10].

Looking at Fig. 2 one can see that HRT results are in very good agreement with Fisher's predictions at high temperatures. In fact, at these temperatures, the effects of a nonzero value for η is very small so that the OZ closure relation is a good approximation of the two-point correlation function $\mathcal{C}^Q(k)$. Conversely below a reduced temperature of about 10^{-2}, HRT predictions already deviate from the correct result. This deviation is an effect of the approximation induced by an OZ closure relation, which leads to the mentioned overestimations of the critical exponents ($\gamma=1.378$, $\nu=0.689$, $\beta=0.345$) [8]. Conversely, at this temperature scale, Dohm equations are already rather accurate.

Figure 3 shows the results for the susceptibility and order parameter below the critical temperature. The asymptotic behavior of the susceptibility turns out to be in good agreement with Dohm predictions, even if small deviations are still present for $\log|t|>-4$. HRT results are not displayed because, as already stated, in this region it gives an identically infinite susceptibility on the coexistence curve.

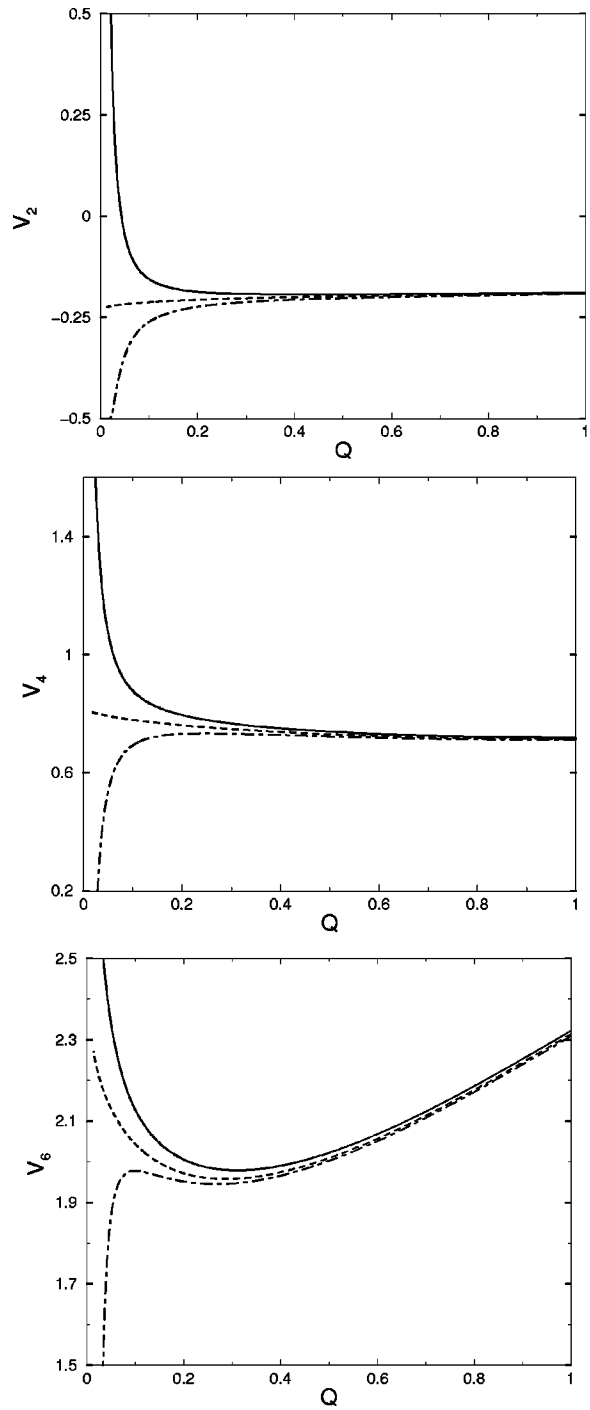

FIG. 1. The expansion coefficients v_2, v_4, and v_6 for the Ising model (Q in units of inverse lattice spacing). Solid line, $t=1.0\times10^{-3}$; dashed line, $t=0$; and the dot dashed line, $t=-1.0\times10^{-3}$. The divergence of coefficients v_2 and v_4 near $Q=0$ is due to the presence of powers of Q in the denominators (10). Exactly at the critical temperature these coefficients tend to a finite limit, otherwise, they diverge to $\pm\infty$, according to whether we are above or below T_c.

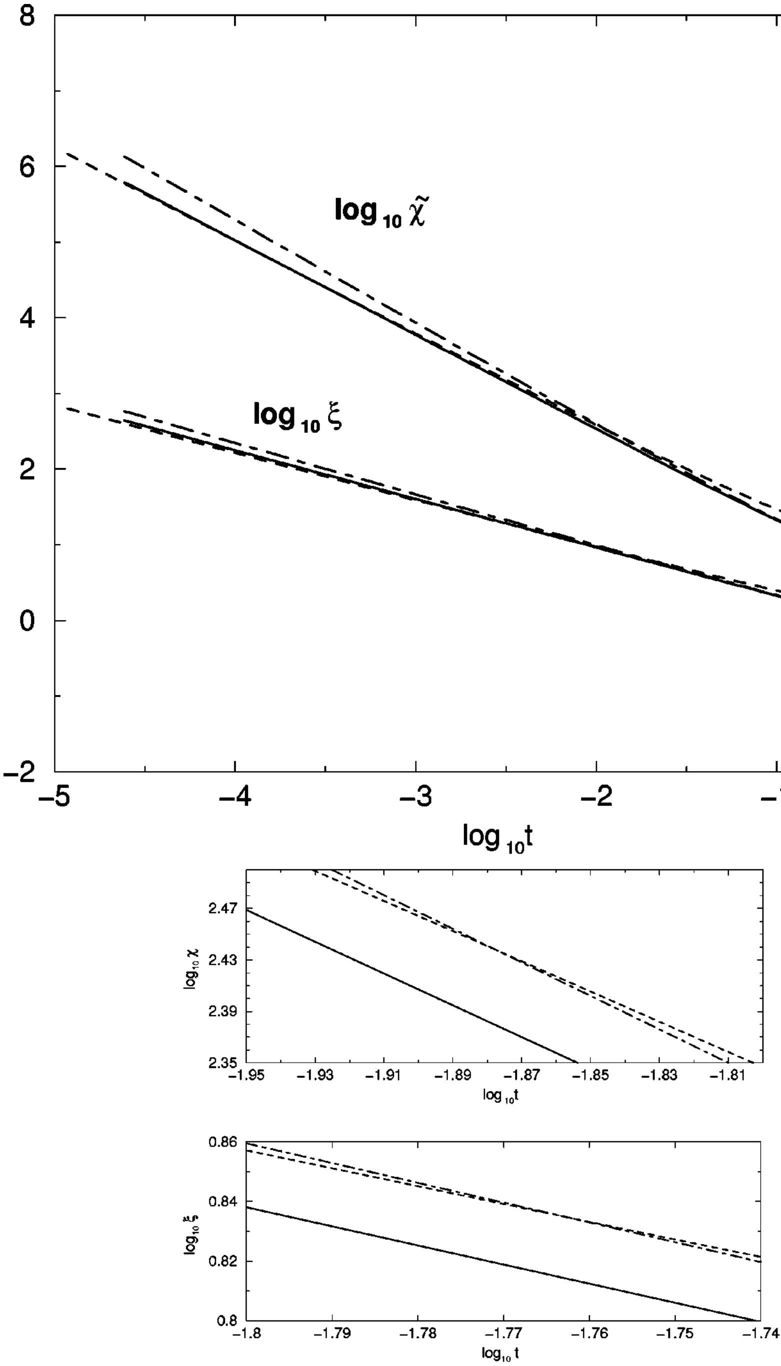

FIG. 2.

FIG. 2. The reduced susceptibility (in units of ideal gas susceptibility) and correlation length (in units of lattice spacing) for the Ising model above T_c. Solid line, Fisher Burford approximants [17]; dot-dashed line, HRT results; and the dashed line, Dohm equations. The new calculation scheme allows us to obtain correct critical exponents. Correlation length is measured in units of lattice spacing.

Dohm results for the order parameter are in good agreement with Fisher's predictions for $\log|t|<-2$.

We believe that the somewhat lower accuracy obtained for the amplitude of the order parameter is due only to the lower accuracy, mentioned above, for the renormalization functions available for this quantity [4].

B. LJ potential

In order to study and to test the validity of the procedure outlined in Sec. II, we applied all the above method to the study of a LJ fluid [19,20]. In this case the reference system is the hard-sphere gas.

As already stated above, the v_6 coefficient, Fig. 4 does not display any minimum and so we have chosen to fix the value of cutoff at $Q=1.0$ as for the Ising model (length units are set by the particle diameter σ). The behavior of the expansion coefficients v_2 and v_4 in the limit $Q\to 0$, is the same as for the Ising model. Figure 5 shows the behavior of the first two odd expansion coefficients v_3 and v_5 [see Eq. (9) and (10)]. Their value at $Q=1.0$ differs from zero because the $\varphi\to-\varphi$ symmetry is recovered only asymptotically close to the critical point. The divergence of v_3 and v_5 at $Q=0$ for $t=0$ is not exactly at the critical density. In the following, we disregard the odd terms even at finite Q be-

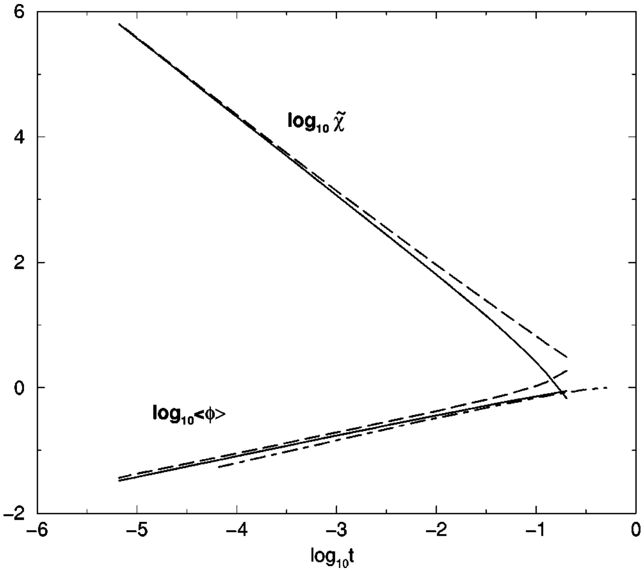

FIG. 3. The reduced susceptibility (in units of ideal gas susceptibility) and magnetization (in the number of spins per site) for the Ising model below T_c. Solid line, the Fisher-Burford-Essam approximants [18]; dot-dashed line, HRT results; and the dashed line, Dohm equations. HRT predictions for susceptibility in this case are identically infinite. In both cases, the agreement with Fisher's extrapolations is very good.

cause their inclusion would require a generalization of the RG equations, which is not yet available.

Even in this case, the final results show no significant dependence on the value of Q in the range $0.5<Q<1.5$.

Unfortunately, comparison with results obtained from other methods, is not as easy as before, because, to the best of our knowledge, Monte Carlo simulation results are not available in the critical region.

We choose to compare only the asymptotic behavior of the physical quantities above and below T_c with the experimental results for Kr [21], results for other rare gases are very similar.

Figure 6 shows the behavior of the isothermal reduced compressibility $[S(0)=nk_BT\kappa_T]$ and the correlation length above T_c. Correlation length amplitude and critical exponents obtained by Dohm equations are in very good agreement with experimental results, and also HRT predictions are in good agreement with experiment unless temperature is very close to T_c. Conversely, the Dohm amplitude for compressibility is not so good as for the Ising model (2) and we find a deviation of about 30%. Also the HRT results underestimate the experimental data over most of the temperature range.

In Fig. 7 the results for the compressibility and the order parameter below critical temperature are presented. As they are above T_c, our results for the susceptibility amplitude, are not in very good agreement with experimental data, while the estimates of the order parameter appear to be accurate.

A possible origin of the discrepancies encountered in the behavior of the compressibility both above and below T_c, derives from the fact that the LJ potential does not describe very well the true intermolecular interaction for a rare gas

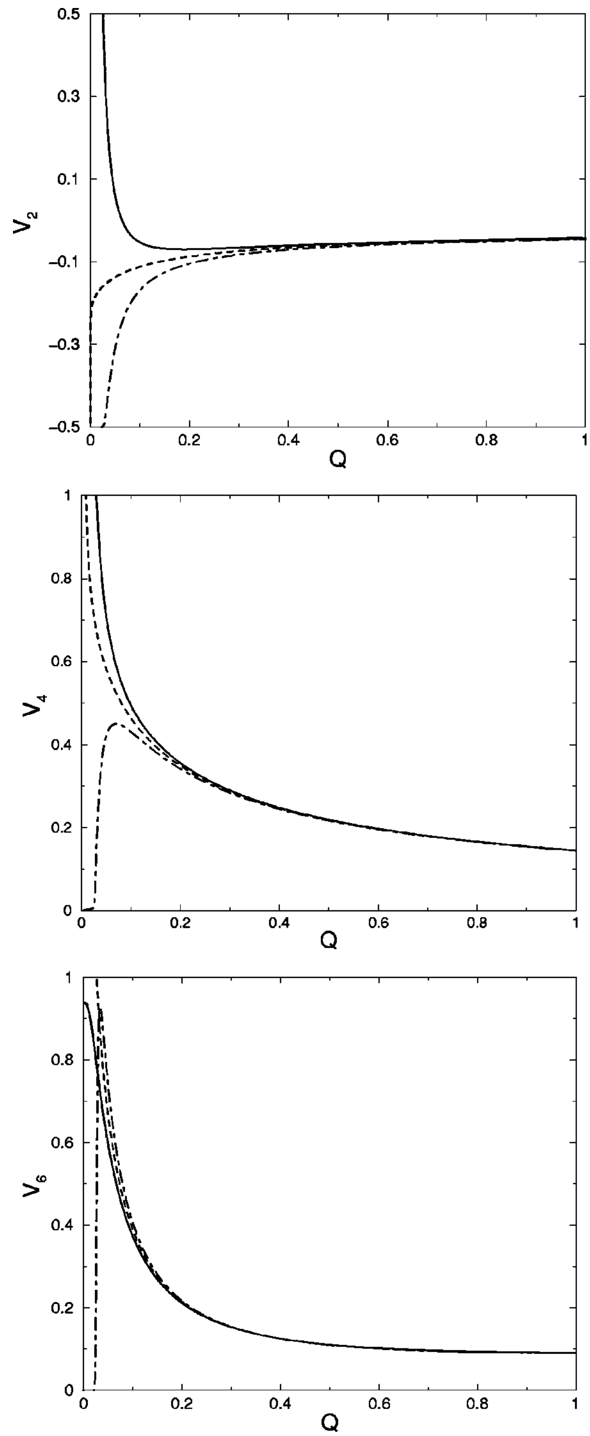

FIG. 4. The expansion coefficients v_2, v_4, and v_6 for the LJ fluid at the same reduced temperatures of the Ising model Fig. 1 (Q in units of inverse lattice spacing). Solid line, $t=1.0\times10^{-3}$; dashed line, $t=0$; and the dot-dashed line, $t=-1.0\times10^{-3}$.

[22]. Another source of inaccuracy can be the presence in a fluid of odd terms. We will comment on this in Sec. III C.

C. Aziz Axilrod-Teller potential

In order to check whether the discrepancies in the susceptibility amplitude presented in Figs. 6 and 7 are due to the

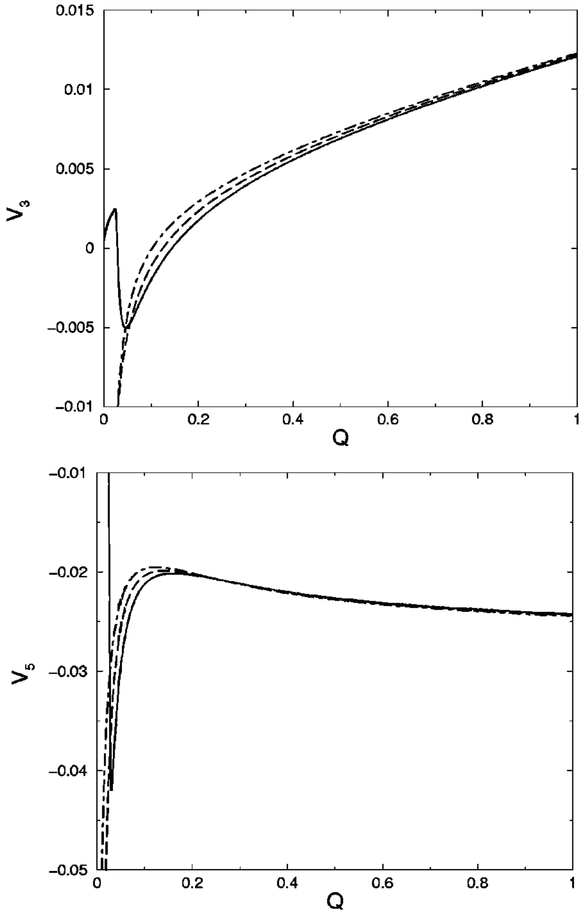

FIG. 5. The behavior of the odd expansion coefficients v_3 and v_5 for the LJ potential (Q in units of inverse lattice spacing). Solid line, $t=1.0\times10^{-3}$; dashed line, $t=0\times10^{-3}$; and the dot-dashed line, $t=-1.0\times10^{-3}$. At $Q=1$, their value differs from zero because invariance $\varphi\rightarrow-\varphi$ is restored only asymptotically close to the critical point. Divergence at $Q=0$ also for $t=0$, is due to the density, which is not exactly at the critical value.

fact that LJ potential does not represent accurately the microscopic interaction of a rare gas, we applied the previously discussed technique to a more accurate potential [22,23] which is believed to describe well the properties of the rare gas. The total interaction is of the form

$$V(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)=\sum_{i<j} v_{Aziz}(|\boldsymbol{r}_i-\boldsymbol{r}_j|)+\sum_{i<j<k} v_{AT}(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k). \tag{22}$$

Here the Aziz potential [24] has been used for the two-body interaction, and the Axilrod-Teller term [25] describes the three-body forces. This last term, which is mostly repulsive, is included in the reference system together with the repulsive part of the Aziz two-body interaction. Thermodynamic and correlation properties of the reference system are calculated using the modified hypernetted chain (MHNC) approximation, extended to treat three-body forces [26]. Details of computation can be found in Ref. [22].

The expansion coefficients (Fig. 8) display the same behavior found for the LJ potentials in the limit $Q\rightarrow0$, and the v_6 term does not present any minimum, so again we choose to fix the value of the matching cutoff at $Q=1.0$ as before.

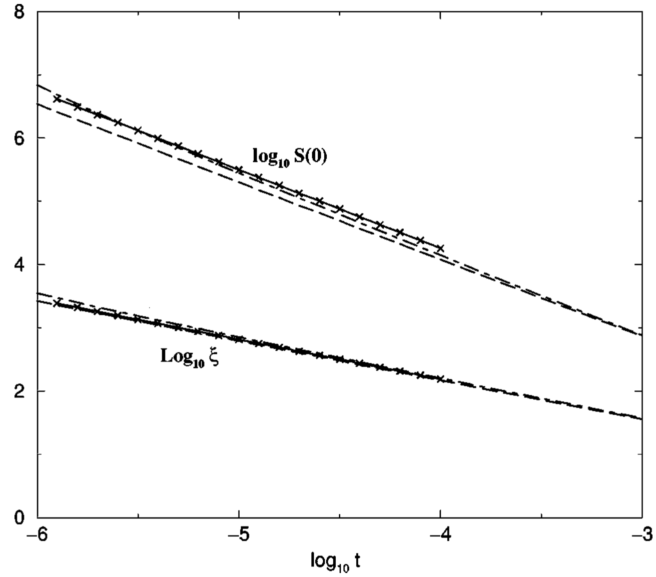

FIG. 6. The reduced isothermal compressibility (in units of ideal gas compressibility) and correlation length (in units of σ) for the LJ potential above T_c. Solid line, experimental data for Kr [21] in the asymptotic region; dot-dashed line, HRT results; the dashed line, Dohm equations. The agreement with susceptibility is not as good as for the Ising model. Discrepancies in the amplitude factors are 30% for susceptibility and 5% for the correlation length.

Odd term coefficients obtained at the same reduced temperatures of LJ are shown in Fig. 9. Nonzero value of these

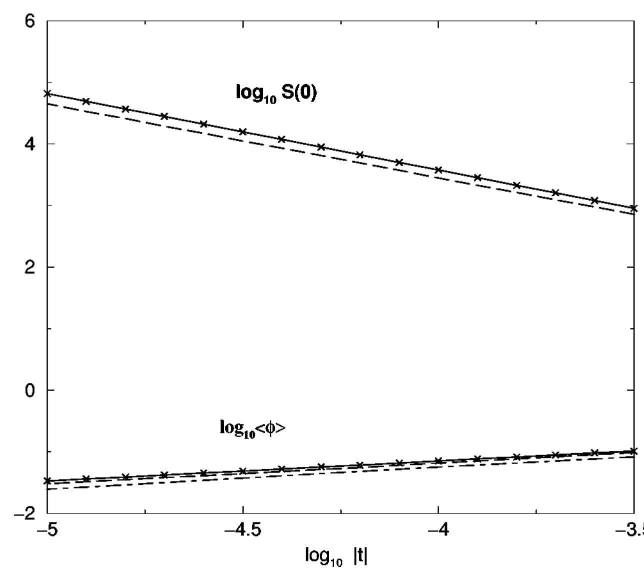

FIG. 7. The reduced isothermal compressibility (in units of ideal gas compressibility) and order parameter (in units of σ^{-3}) for LJ potential below T_c. Solid line, experimental data for Kr [21]; dot-dashed line, HRT results; and dashed line, Dohm equations. Experimental data for Kr are valid only in the asymptotic region. The amplitude factor for susceptibility has been derived from the amplitude factor above T_c using the universal ratio between these two quantities which is 4.8. Discrepancies for the susceptibility amplitude are 30%, while for the order parameter they are 10%.

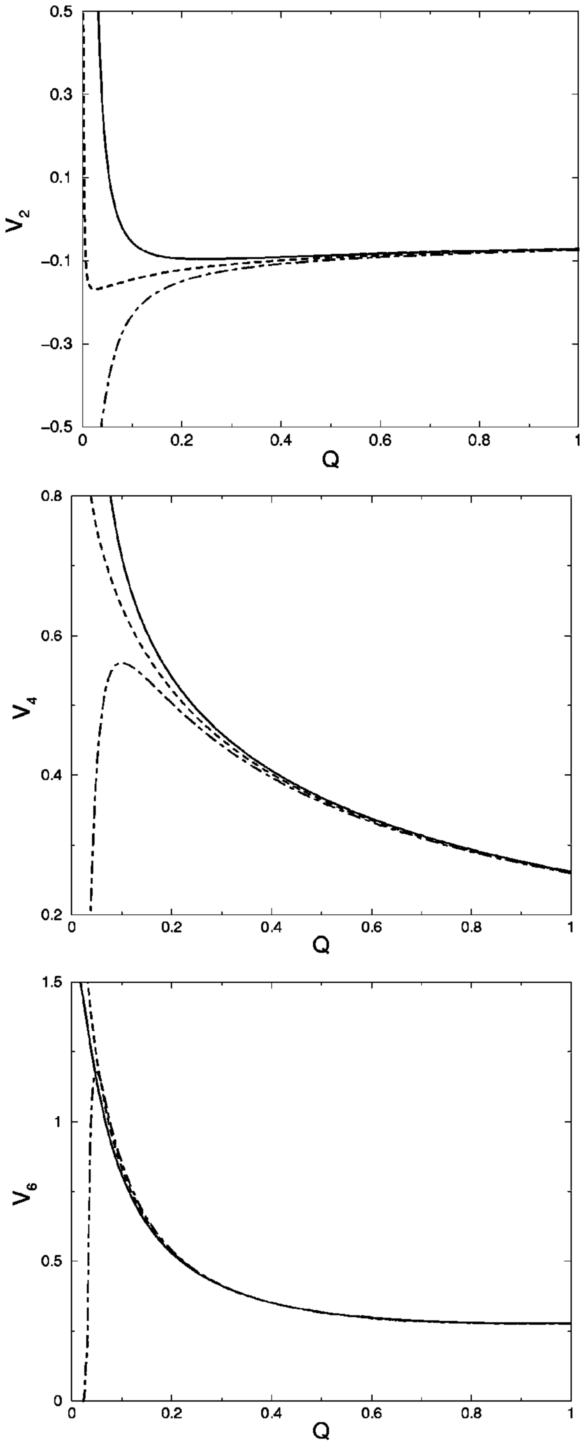

FIG. 8. The expansion coefficients v_2, v_6, and v_6 for the Aziz Axilrod-Teller potential (Q in units of inverse lattice spacing). The reduced temperature is the same Figs. 1 and 4. Solid line, $t=1.0\times 10^{-3}$; dashed line, $t=0$; and the dot-dashed line, $t=-1.0\times 10^{-3}$. As for LJ (4) there is no minimum is the v_6 coefficient behavior. The matching procedure is done at $Q=1.0$. The behavior of expansion coefficients resembles that of Fig. 4 near $Q=0$.

coefficients at $Q=1.0$ should be noted, while the divergence at $t=0$ is as before due to be only approximately at the critical density.

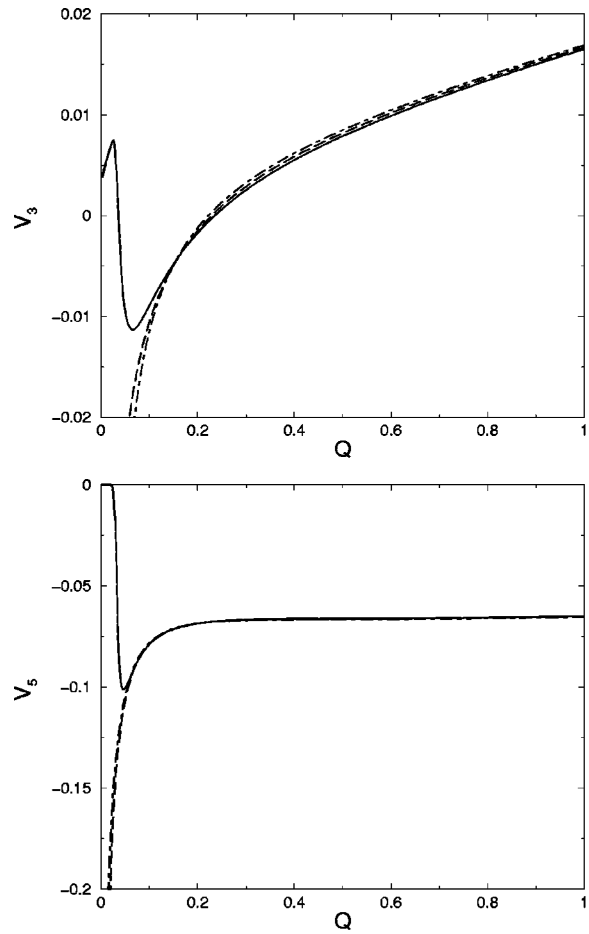

FIG. 9. The odd expansion coefficients for the Aziz potential (Q in units of inverse lattice spacing). Reduced temperatures are the same for Fig. 5. Solid line: $t=1.0\times 10^{-3}$; dashed line, $t=0$; and the dot-dashed line, $t=-1.0\times 10^{-3}$; Here as for the LJ case of Fig. 5, divergencies at $Q=0$ for the critical temperature are due to be not exactly at the critical density.

The asymptotic region results above T_c are shown in Fig. 10. Comparison is made as before with the experimental data for Kr [21]. As can be seen, agreement for isothermal compressibility is improved (cf. Fig. 6) but correlation length predictions are of slightly worse quality than that of LJ.

Similar considerations can be done for the results below T_c, presented in Fig. 11, where results for isothermal compressibility are not very precise (even if better than the LJ potential of Fig. 7; discrepancies in the amplitude factor are now about 12%) whereas predictions for the order parameter are good.

D. Terms beyond the φ^4 model

As stated in the previous sections, the good results obtained for the Ising model are not encountered in the susceptibility of the fluid models. The discrepancies encountered could be ascribed to the fact that, for fluid models, the effective Hamiltonian (9) should include odd power terms. These terms disappear only at the critical point ($Q=0$) when invariance $\varphi\to-\varphi$ is restored. But at $Q=1.0$, their presence can affect the final results.

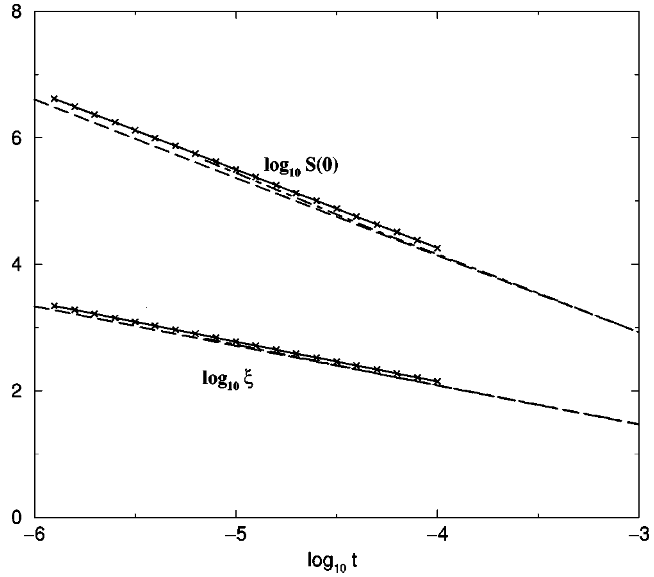

FIG. 10. The reduced isothermal compressibility (in units of ideal gas compressibility) and correlation length (in units of σ) for the Aziz Axilrod-Teller potential above T_c. Solid line, experimental data for Kr in the asymptotic regime [21]; dot-dashed line, HRT results; and the dashed line, Dohm equations. The agreement with susceptibility is quite better than that obtained for the LJ fluid (discrepancy in the amplitude factor is now of 12%); conversely results for the correlation length are just a little worse (accuracy for the amplitude factor is about 10%).

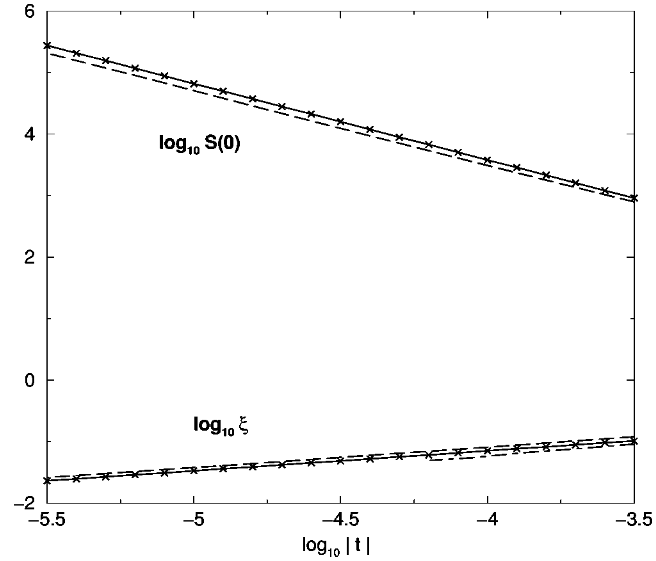

FIG. 11. The reduced isothermal compressibility (in units of ideal gas compressibility) and order parameter (in units of σ^{-3}) for the Aziz Axilrod-Teller potential below T_c. Solid line, experimental data for Kr in the asymptotic regime; dot-dashed line, HRT results; and the dashed line, Dohm equations. The error on the amplitude factor are about 12% and of 10% for susceptibility and order parameter, respectively.

In order to test the effective relevance of the terms neglected from the Hamiltonian of Eqs. (9) and (10) we compared the second derivative of the free energy ($\partial^2 A/\partial\rho^2$) obtained from the HRT integration at $Q=1.0$ with the polynomial parametric representation obtained using the expansion coefficients of Eq. (10) evaluated at the same cutoff. The results of this test are presented in Figs. 12–14. Figure 12 shows that the free energy of the Ising model is well approximated by a φ^4 Hamiltonian (at least for low magnetizations); the φ^6 term begins to be important only for magnetization greater then 0.1. Figure 13(a) instead clarifies the role of odd terms for LJ potentials. It can be seen that, even at densities close to the critical density, the free energy is not well represented by a φ^4 Hamiltonian because of the presence of the odd terms. However, it is possible to eliminate the effects of the first odd term φ^3 defining the critical density as the density at which $\partial^2 A/\partial^2\rho$ has its minimum. Figure 13(b) shows the results obtained with this redefinition of the critical density, which must be lowered by 3%. It is also possible to note that the second odd term φ^5 gives very little correction. Figure 14 shows the same of Fig. 13 for the Aziz potential; in this case the critical density is lowered by 1.5%. The contribution of the φ^5 term is greater than before.

We performed the integration of the Dohm equation, evaluating the expansion coefficients of Eq. (10) at this effective critical density, both for LJ and Aziz potentials, but the results for the physical quantities are almost unchanged by this redefinition. We conclude that the φ^3 term is not responsible for the lower quality of the results for a fluid. On the other hand, comparison of the contributions to the effective Hamiltonian of terms beyond φ^4 for the Ising model (Fig. 12) and for the fluid models (Figs. 13 and 14) shows that these terms are more relevant for fluids model. The relative importance of the φ^6 term is similar for the two models of a fluid and larger than in the case of the Ising model. In addition, the φ^5 term is very small for the LJ potential, but it is quite significant in the case of the Aziz potential with three-body forces, and this is in agreement with the general

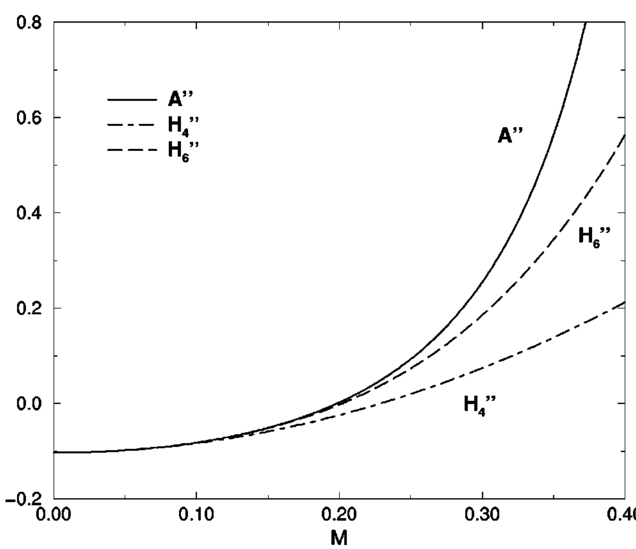

FIG. 12. The free energy for the Ising model $A'' = \partial^2(-\beta A/V)/\partial M^2$ is compared with the polynomial parametric representation obtained for φ^4 (H_4) and φ^6 (H_6) Hamiltonians. The contribution of the φ^6 term is negligible for magnetization lower than 0.1.

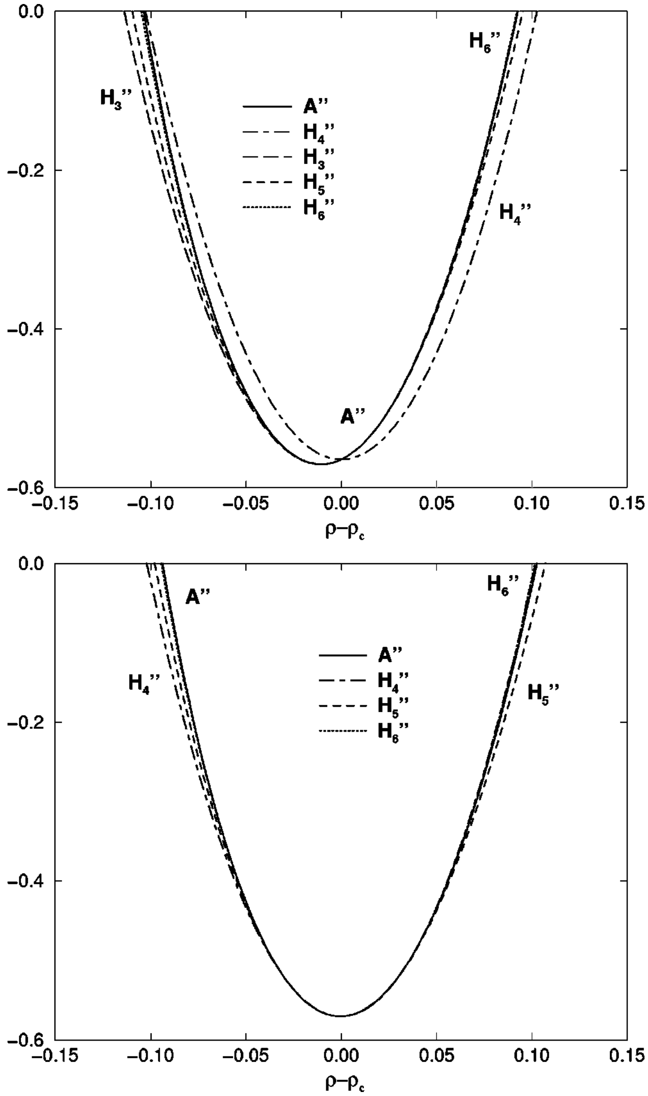

FIG. 13. The free energy for the LJ model $A''=\partial^2(-\beta A/V)/\partial\rho^2$ (ρ in units of σ^{-3}). The comparison is made with polynomial parametric representations for the theories: $H_4=v_2(\rho-\rho_c)^2+v_4(\rho-\rho_c)^4$, $H_3=v_2(\rho-\rho_c)^2+v_3(\rho-\rho_c)^3+v_4(\rho-\rho_c)^4$, $H_5=v_2(\rho-\rho_c)^2+v_3(\rho-\rho_c)^3+v_4(\rho-\rho_c)^4+v_5(\rho-\rho_c)^5$, and $H_6=v_2(\rho-\rho_c)^2+v_3(\rho-\rho_c)^3+v_4(\rho-\rho_c)^4+v_5(\rho-\rho_c)^5+v_6(\rho-\rho_c)^6$. In the upper figure, expansion coefficients are evaluated at the HRT critical density. Odd terms make it impossible to fit the free energy with the H_4 Hamiltonian. In the figure, expansion coefficients are evaluated at the effective critical density, where A'' has a minimum.

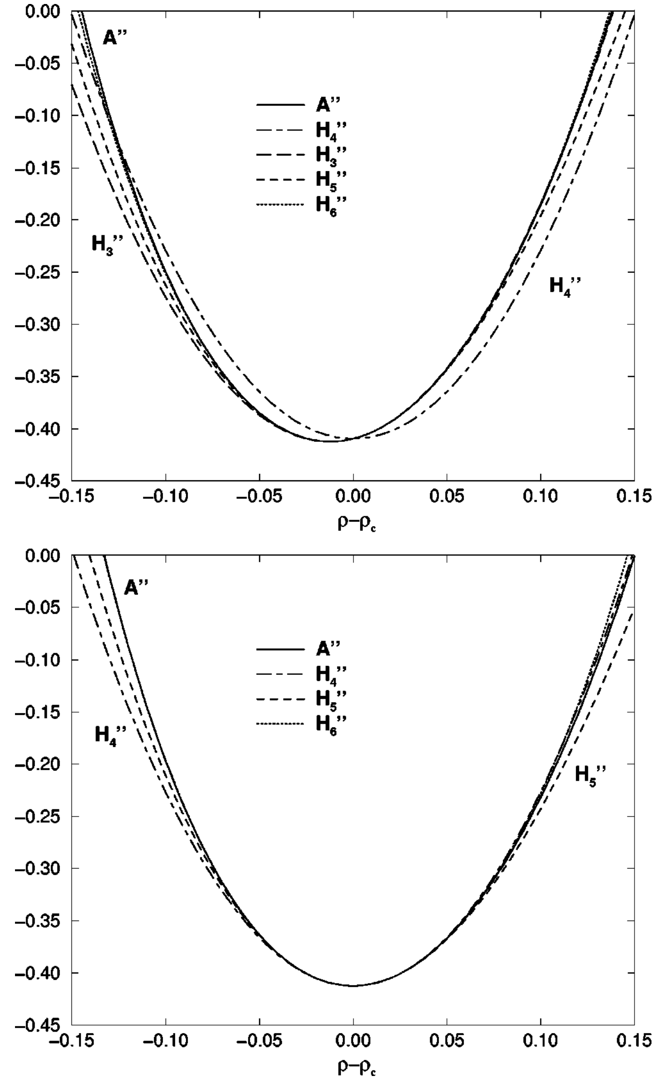

FIG. 14. The free energy for the Aziz potential (ρ in units of σ^{-3}). Hamiltonians have the same meaning for Fig. 13. In this case the $(\rho-\rho_c)^5$ term is more important than for the LJ potential.

understanding of the role of three-body forces on criticality [28].

IV. CONCLUSIONS

We have developed a method that allows to obtain a quantitative link between HRT, which is an implementation of Wilson's momentum shell renormalization group, and RG equations, which instead are based on the minimal subtraction scheme. This method requires the identification of a momentum scale Q_0, where the microscopic (HRT) and the coarse grained (φ^4) theories match. It is reassuring to observe that indeed a range of values of the cutoff exists where this matching is possible and that the results do not strongly depend on the choice of Q_0.

The combined use of these two methods allowed us to obtain results for physical quantities above and below the critical temperature for the three models presented in Sec. III. In particular, susceptibility and correlation length predictions below T_c, represent an extension of the HRT results.

Remarkably, the application of this method to the Ising model led to results that are in very good agreement with series expansion predictions, both above and below the critical temperature. The application of this method to fluid models is less satisfactory. The results for correlation length and order parameter are in good agreement with experimental results for krypton, but the results for compressibility when the LJ potential is used, are not very good. When a better representation of the interatomic potential is used, the agreement with experimental data in the critical region improves for the compressibility, but the correlation length is less accurate. Globally the quality of the results for a fluid model is significantly inferior to that for the Ising Model.

As a source of inaccuracy in the case of a fluid, two possibilities can be considered. The first one is that the long-wavelength density fluctuations in a realistic fluid model, are only approximatively described by a φ^4 theory. In fact we find that, even within LPA, there are further interactions to be retained in the effective Hamiltonian expansion (9), see Figs. 16 and 19. The tests performed in Figs. 13 and 14 showed us that even the redefinition of the critical density, which allows us to minimize the effects of the lowest odd term, gives no significant improvements on the physical quantities. Furthermore, the crossover phenomena for fluids are much more complicated than for the Ising model [27], so the matching between HRT and Dohm equations may be less accurate. The second possibility concerns the interparticle potentials, which may describe the true interaction between the fluid particles in the critical region only approximatively. In addition there is an interplay between interatomic interaction and higher-order terms in the effective Hamiltonian. It is known [22] that the LJ potential is not an accurate model of the interatomic interaction, but when the more accurate Aziz potential is used, it is also necessary to introduce three-body forces. In this last case, the φ^5 term becomes much more relevant [28] and it is plausible that what we gain with the better modelization of the interatomic potential is lost by the less accurate representation of the effective Hamiltonian in terms of the φ^4 model.

We hope that this paper will motivate the development of new techniques to deal with more complex field theories, which include external fields and higher-order terms in the expansion of the effective potential (9). This would allow us to get information about other physical quantities like the magnetization along the critical isotherm, and to hopefully improve the agreement with experimental data for fluid models.

In particular, in Ref. [29] is discussed a theory that allows to obtain susceptibility, correlation length, and order parameter even in the preasymptotic region. Monte Carlo simulations of the Ising model are in good agreement with results predicted by this theory, as shown in Refs. [30,31]. However the details of the specific thermodynamic model enter in this theory only through parameters, which cannot be predicted by the theory itself, but must be derived from other methods. It may be interesting to use HRT to derive these parameters in order to try to improve the results obtained for the fluid models discussed.

Finally, the study of more sophisticated closure relations to the HRT equations, should also improve the accuracy in the determination of the initial conditions of the RG equations.

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