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INTERFACE TENSION IN THREE-DIMENSIONAL SYSTEMS FROM FIELD THEORY

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In liquid mixtures or analogous binary systems at low temperatures the pure phases may coexist, separated by an interface. The interface tension vanishes according to $\sigma = \sigma_0(1 - T/T_c)^{\mu}$ as the temperature T approaches the critical point from below. Similarly, the correlation length diverges as $\xi = \xi_0^+(T/T_c - 1)^{-\nu}$ in the high-temperature region. For three-dimensional systems the dimensionless product $R_+ = \sigma_0(\xi_0^+)^2$ is universal. We calculate its value in the framework of field theory in $d = 3$ dimensions without recourse to the ϵ-expansion. The result $R_+ = 0.39 \pm 0.03$ is in agreement with experimental data.

1. Introduction

Various binary liquid mixtures exhibit the phenomenon of phase separation (see refs. [1, 2]). Below a certain critical temperature T_c the two liquids cannot be mixed completely. An interface forms which separates two phases with different relative concentrations. It is associated with an interface tension τ which varies with the temperature T. For interfaces in other critical binary systems, e.g. for liquid–gas coexistence, the same considerations apply. For later convenience we introduce the reduced interface tension

$$\sigma = \tau/kT\,, \tag{1}$$

where k is Boltzmann's constant. As T increases towards T_c the interface becomes more and more diffuse and at T_c the interface tension vanishes according to the scaling law

$$\sigma \sim \sigma_0 t^{\mu}\,, \tag{2}$$

where

$$t = \left| \frac{T - T_c}{T_c} \right|, \tag{3}$$

and σ_0 is the critical amplitude of the interface tension. The experimental results for the critical index μ are consistent with the universal value [3–6]

$$\mu = 1.26 \pm 0.01 . \tag{4}$$

For temperatures above T_c a homogeneous mixture can be produced. The correlation length ξ in this mixture diverges as T approaches T_c from above according to

$$\xi \sim \xi_0^+ t^{-\nu} . \tag{5}$$

The experimental values for the critical exponent ν [7–9] are consistent with the prediction from the renormalization group [10],

$$\nu = 0.630 \pm 0.002 . \tag{6}$$

In the low-temperature phase a correlation length and corresponding amplitude ξ_0^- can also be defined but is not easily accessible experimentally.

In three dimensions the exponents μ and ν are related through Widom's scaling law [3, 11],

$$\mu = 2\nu , \tag{7}$$

which is a consequence of the scaling hypothesis. Furthermore, the dimensionless product of critical amplitudes

$$R_+ = \sigma_0 (\xi_0^+)^2 , \tag{8}$$

is expected to be a universal number although the amplitudes themselves vary considerably for different substances [12, 13]. The constant R_+ has been determined experimentally for a number of mixtures and simple fluids [5, 6, 14]. The results can be summarized by

$$R_+ = 0.38 \pm 0.02 \quad (\text{exp.}) . \tag{9}$$

On the other hand, first Monte Carlo calculations for the interface tension in the three-dimensional Ising model [15] gave rise to the smaller value $R_+ \approx 0.24$. The same quantity was calculated by Pant [16] and Brézin and Feng [17] in the framework of quantum field theory by means of the ϵ-expansion, where $d = 4 - \epsilon$ is the number of dimensions of space. Evaluated at $\epsilon = 1$ the result is 0.14 to first order and 0.2 to second order in ϵ. The discrepancy between the experimental and theoretical numbers gave rise to worry among experimentalists and caused the reconsideration of experiments in view of possible systematic errors [5, 6, 14]. The analysis, however, resulted in a confirmation of the experimental value.

A recent study of the Ising model led to a reconciliation of the Monte Carlo value for R_+ with the experimental one [18]. With the help of a finite-size scaling analysis Mon obtained

$$R_+ = 0.36 \pm 0.01 \quad (\mathrm{MC}) . \tag{10}$$

This result has been confirmed by Meyer-Ortmanns and Trappenberg [19]. To measure the interface tension the latter authors employ a new method, used in ref. [20] for the four-dimensional Ising model, which reduces the finite-size effects on σ.

The situation described above calls for a new field-theoretical treatment of the problem. In this article the results of such an investigation are presented.

2. Interface tension from renormalized field theory

The framework for field-theoretic investigations of critical phenomena is euclidean ϕ^4-theory. The scalar field $\phi(x)$ represents the local order parameter which in our case is proportional to the difference of the concentrations of the two fluids.

Studies of the properties of interfaces near criticality are confronted with two problems. The first one is more general and also concerns bulk quantities. Due to infrared divergences in $d = 3$ dimensions it is not possible, in contrast to the four-dimensional case, to construct the critical, i.e. massless, theory within perturbation theory. This led to the introduction of the ϵ-expansion [21] (for a review see ref. [22]), whee the theory is considered in $4 - \epsilon$ dimensions and all calculations are effectively done in the four-dimensional theory. This difficulty, however, has been overcome in refs. [10, 23]. There the massive three-dimensional theory is considered in renormalized perturbation theory. The renormalized coupling g_{R} is dimensionful and the perturbation expansion actually goes in powers of the dimensionless variable

$$u_{\mathrm{R}} = g_{\mathrm{R}}/m_{\mathrm{R}} , \tag{11}$$

where m_{R} is the renormalized mass. This indicates the infrared problem for the critical theory. But the variable u_{R} has a finite limit u_{R}^* if one approaches the critical point. Thus information about the critical theory can be obtained by evaluating the expansions at u_{R}^*. With the help of series summation techniques this has led to very precise estimates of critical exponents.

Concerning the critical behaviour of interfaces in three or less dimensions another infrared problem shows up which is due to the roughening transition [24]. Near the critical point long-wavelength fluctuations of the interface lead to a delocalization of the interface, whose width diverges logarithmically with its diameter [25]. This manifests itself in the form of infrared divergences in calcula-

tions of the interface profile [26–28]. Therefore, field-theoretic calculations of interface properties have so far been done in the ϵ-expansion [16, 17].

The interface tension, however, remains finite even in the presence of the roughening phenomenon. This fact is clearly visible in the case of the two-dimensional Ising model, where the interface is always rough, but its tension has a finite value already determined by Onsager [29]. It should thus be possible to calculate the interface tension directly in three dimensions without recourse to the ϵ-expansion. This is the approach which will be taken in the following.

The bare lagrangian of euclidean ϕ^4-theory in the broken symmetry phase is written as

$$\mathscr{L} = \tfrac{1}{2}\partial_\mu \phi_0 \partial^\mu \phi_0 + V(\phi_0), \tag{12}$$

where the double-well potential

$$V(\phi_0) = -\frac{m_0^2}{4}\phi_0^2 + \frac{g_0}{4!}\phi_0^4 + \frac{3}{8}\frac{m_0^4}{g_0} = \frac{g_0}{4!}\left(\phi_0^2 - v_0^2\right)^2 \tag{13}$$

has its minima at

$$\phi_0 = \pm v_0 = \pm\sqrt{3m_0^2/g_0}\,. \tag{14}$$

The parameters are defined such that the value of the potential at its minima is zero and m_0 is the bare mass. The renormalized mass

$$m_R = 1/\xi^{(2)} \tag{15}$$

is the inverse of the second moment correlation length. It is defined together with the wave-function renormalization Z_R through the small-momentum behaviour of the propagator:

$$G(p)^{-1} = \frac{1}{Z_R}\left\{m_R^2 + p^2 + O(p^4)\right\}. \tag{16}$$

In the critical region m_R is within the accuracy considered here numerically indistinguishable from the "true" mass m, which equals the inverse true correlation length $1/\xi$ [30]. The renormalized vacuum expectation value of the field is

$$v_R = Z_R^{-1/2} v\,, \tag{17}$$

where v is the expectation value of the field ϕ_0. For the renormalized coupling I

adopt the definition

$$g_R = 3\left(m_R^2/v_R^2\right), \tag{18}$$

which is very convenient in the low-temperature phase [31, 32].

Now I turn to the consideration of the interface tension. A corresponding investigation in the case of $d = 4$ dimensions has been made in ref. [33] where more details about the method can be found. The basic idea behind the calculation is a relation between the interface tension and the tunneling correlation length. Let the hamiltonian H be the generator of translations along the x^0-coordinate. The other coordinates are called x^1 and x^2. We consider a cylinder-type geometry, where the cross section perpendicular to x^0 is quadratic of area $L \times L$ and the fields obey periodic boundary conditions. Then H has a unique ground state which is symmetric under the reflection $\phi \to -\phi$. Separated from the ground state by a small energy splitting ΔE is an antisymmetric state. This means that the degeneracy of the infinite volume ground states is lifted. The energy splitting ΔE is due to tunneling and its inverse is called the tunneling correlation length ξ_L. Its area dependence has been predicted [34–36] to be of the form

$$\Delta E = C \exp(-\sigma L^2), \tag{19}$$

where σ is the interface tension. One sees that tunneling effects vanish very rapidly with increasing area.

The energy splitting can be calculated in a semi-classical calculation including one-loop effects. To this end one considers the tunneling amplitude which is given by the euclidean path integral with boundary conditions

$$\phi(x) \longrightarrow \begin{cases} v_0, & x^0 \to \infty \\ -v_0, & x^0 \to -\infty \end{cases} \tag{20}$$

and evaluates it by means of the saddle point approximation. The path integral is dominated by a classical solution, the so-called "kink":

$$\phi_c(x) = \sqrt{\frac{3m_0^2}{g_0}} \tanh\left(\tfrac{1}{2}m_0(x^0 - a)\right) \tag{21}$$

with classical action

$$S_c = 2\frac{m_0^3}{g_0}L^2. \tag{22}$$

a is a free parameter specifying the location of the kink. In the language of

statistical mechanics this solution represents a bare interface (fluctuations are still neglected) which separates the two phases corresponding to $\phi(x) = v_0$ and $\phi(x) = -v_0$ respectively. S_c is then the energy of the interface.

In the one-loop approximation the quadratic fluctuations around the classical solution are taken into account as a gaussian integral. For fluctuations

$$\phi = \phi_c + \eta ,$$

the quadratic part of the action is given by

$$S = S_c + \frac{1}{2} \int d^3x \, \eta(x) M \eta(x) + O(\eta^3) \tag{23}$$

with the fluctuation operator

$$M = -\partial_\mu \partial^\mu + m_0^2 - \tfrac{3}{2} m_0^2 \cosh^{-2}\left(\tfrac{1}{2} m_0 (x^0 - a)\right). \tag{24}$$

M has a zero mode corresponding to translations of the kink or shifts of the parameter a, which has to be treated separately by the method of collective coordinates [37]. Taking into account also all contributions from non-interacting multi-kink configurations, which exponentiate, the result for the energy splitting is

$$\Delta E = 2 e^{-S_c} \left(\frac{S_c}{2\pi} \right)^{1/2} \left| \frac{\det' M}{\det M_0} \right|^{-1/2} , \tag{25}$$

where det' is the determinant without zero modes and

$$M_0 = -\partial_\mu \partial^\mu + m_0^2 . \tag{26}$$

The factor $S_c^{1/2} \sim L$ is due to the zero mode. The determinant, which represents a one-loop effect, leads to the following three types of contributions. First of all it produces precisely those counterterms which are required to convert the unrenormalized parameters appearing in eq. (25) into the renormalized ones. Moreover it yields an additional factor L^{-1}. Finally it gives a one-loop correction to the term proportional to L^2 in the exponential. Using the techniques of ref. [33] the determinants can be evaluated analytically. Omitting the details of the calculation, which are analogous to those in ref. [33], the final result is

$$\Delta E = C \exp\{-\sigma(L) L^2\}, \tag{27}$$

with

$$C = 4\frac{\Gamma(3/4)}{\Gamma(1/4)}\sqrt{\frac{2}{u_R}}\, m . \tag{28}$$

The interface tension σ has a negligible exponentially small L-dependence. Its value at $L = \infty$ is

$$\sigma_\infty = 2\frac{m^2}{u_R}\left(1 - \frac{u_R}{4\pi}\left(\frac{39}{32} - \frac{15}{16}\log 3\right) + O(u_R^2)\right). \tag{29}$$

3. Conclusion

Since m is the inverse of the correlation length in the low-temperature phase, the result of sect. 2 immediately leads to an expression for the amplitude product,

$$R_- = \sigma_0(\xi_0^-)^2 = \frac{2}{u_R^*}\left(1 - \frac{u_R^*}{4\pi}\left(\frac{39}{32} - \frac{15}{16}\log 3\right) + O(u_R^{*2})\right). \tag{30}$$

In order to get a numerical estimate we have to evaluate it at the fixed point value u_R^* of u_R. In the language of statistical physics u_R^* can be expressed as the universal amplitude ratio

$$u_R^* = \frac{3C_-}{(\xi_0^{(2)-})^3 B^2}, \tag{31}$$

where B and C_- are the critical amplitudes of the magnetization and low-temperature susceptibility of an Ising type system respectively. Using the results of refs. [30, 38, 39] one finds

$$u_R^* = 15.1 \pm 1.3 . \tag{32}$$

This yields

$$R_- = 0.1024 \pm 0.0088 . \tag{33}$$

The one-loop contribution amounts to 22% of the leading term and we may assume that the next order yields a correction of a few percents. The desired quantity

$$R_+ = \left(\frac{\xi_0^+}{\xi_0^-}\right)^2 R_- \tag{34}$$

is finally obtained with the help of the conversion factor [30, 40]

$$\frac{\xi_0^+}{\xi_0^-} = 1.96 \pm 0.03\,, \tag{35}$$

and reads

$$R_+ = 0.39 \pm 0.03\,. \tag{36}$$

The discrepancy between the experimental, eq. (9), and field-theoretic numbers thus appears to be resolved.

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