PATH INTEGRALS FOR SELF-AVOIDING RANDOM LOOPS AND SURFACES

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ABSTRACT

I point out the relevance of self-avoiding random loops and surfaces to many physical systems and show how their partition function can be formulated as path integrals over unitary real or Ising field variables. These can easily be studied by analytic and Monte Carlo methods.

[+] On Sabbatical from: Institut für Theorie der Elementarteilchen, Freie Universität Berlin, Arnimallee 14, 1000 Berlin 33, Germany.

[*] Supported in part by Deutsche Forschungsgemeinschaft under grant no. Kl 256.

The transitions in many physical systems are dominated by the unlimited growth of line-like or surface-like geometrical objects. The most thoroughly studied example for the first case is the superfluid phase transition where vortex lines proliferate and cause the well-known λ - peak in the specific heat. The evidence that this peak is really caused by random lines is given by the Villain model, which is precisely equivalent to a sum over such lines, and which shows the same peak in the specific heat (see Fig. 1). The process of crystal melting is another important example. Here it is the defect lines, whose growth causes the breakdown of crystalline order. All these systems are discussed in detail in Ref. 1.

The above mentioned lines are characterized by the property that they are non-self-backtracking which means that a line cannot fold back onto itself (since the folded piece would annihilate and must not be counted as a physical configuration).

In this lecture I want to focus on a third type of process where line-like objects play an important role, namely polymerization, in particular, the polymerization of sulfur. Around 115°C, sulfur exists mainly in the form of S_8 rings. As the temperature approaches a critical point of $T_c \approx 160°C$, the rings break open and join ends to form infinitely long chains. The specific heat has a peak shown in Fig. 1. Such line-like objects are self-avoiding. At every place there can be at most one line element.

In all such line systems, the phase transition occurs when the entropy per line element times temperature becomes larger than the energy per line element.

In order to study ensembles of self-avoiding chains it was proposed, by Rys and Helfrich$^{2)}$ and Wheeler and Pfeuty$^{3)}$, to use a spin model of n components, with only one of them coupled in an Ising like fashion, calculate all results as a function of n and let $n \rightarrow o$ at the end. Besides the fact that the high-temperature series contains unphysical configurations (one-link closed chains going forward and backward on the same link) and spurious "zero-link objects"3,4) this model has the unfortunate drawback that it cannot be simulated on a computer via Monte Carlo techniques. By using path integral methods, T. Hofsass and I were able to find a much more manageable model3) whose partition function, on a simple cubic lattice, reads

$$Z = \prod_{\vec{x}} \Big[\int_{-\pi}^{\pi} \frac{d\theta(\vec{x})}{2\pi} \left(1 + u^{*2}(\vec{x})\right) \Big] \prod_{\vec{x},\vec{i}} \left[1 + v\, u(\vec{x}) u(\vec{x}+\vec{i}) \right] \tag{1}$$

where $u(\vec{x}) = e^{i\theta(\vec{x})}$ are pure phase variables at each site $\vec{x}$ and v is the Boltzmann factor $\exp(-\varepsilon/T)$ (fugacity) associated with each occupied link i. This formula is easy to understand. The right-hand product gives rise to all possible chain elements across the links from $\vec{x}$ to $\vec{x} + \vec{i}$ (at most one per link) and the integral over $d\theta\,(1 + u^{*2})$ either annihilates a chain element (1) or joins up its ends with a neighbor (u^{*2}). It is easy to see that the Ising model can also be written in this form with $1 + u^{*2}$ being replaced by the infinite series $(1 + u^{*2} + u^{*4} + \ldots)$ and $v = \operatorname{th} \beta$. This accounts for the fact that in the high temperature (small β) series of the Ising model, lines can cross on a site from all directions. Since each link can be occupied at most once, this number is limited by D such that, in D dimensions, the infinite series may be truncated after $(u^*)^{2D}$ without any harm.

Another representation of the partition function is obtained by observing that $\int_{-\pi}^{\pi} d\theta\, (2\pi)^{-1} u^{*n} u^m$ is the same as $\int_{-\infty}^{\infty} du \int_{-i\infty}^{i\infty} \frac{d\alpha}{2\pi i} \frac{1}{n!} \alpha^n u^m e^{-\alpha u}$. Hence the partition function can also be written in terms of real variables as

$$Z = \prod_{\vec{x}} \Big[\int_{-\infty}^{\infty} du(\vec{x}) \int_{-i\infty}^{i\infty} d\alpha(\vec{x}) (2\pi i)^{-1} \Big] \prod_{\vec{x}} \left(1 + \tfrac{1}{2} \alpha(\vec{x})^2\right) \prod_{\vec{x},\vec{i}} \left(1 + v\, u(\vec{x}) u(\vec{x}+\vec{i})\right) \tag{2}$$

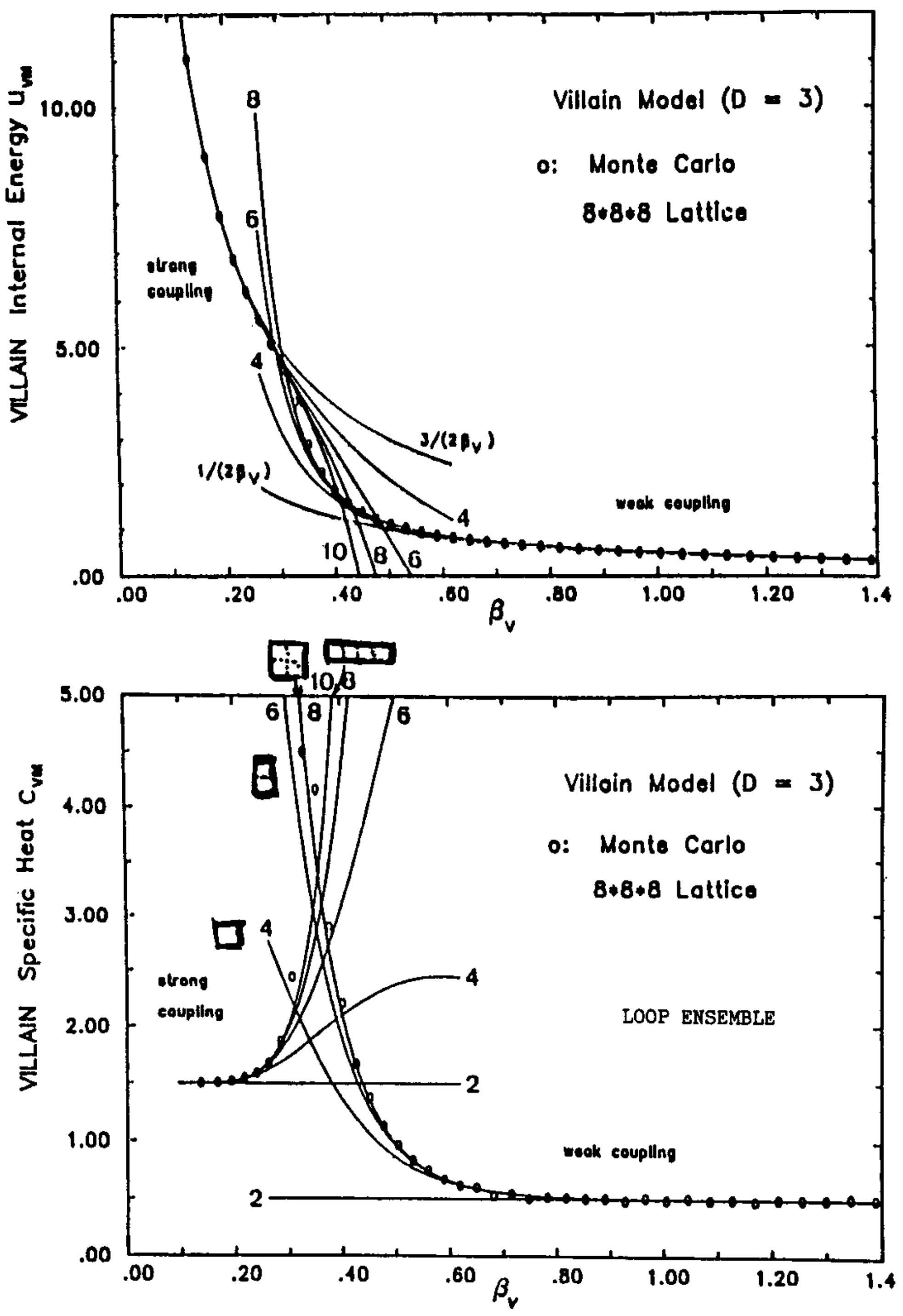

Fig. 1 Internal energy and specific heat of non-self-backtracking random loops as calculated from the Villain model. (From W. Janke and H. Kleinert, Berlin preprint, 1985)

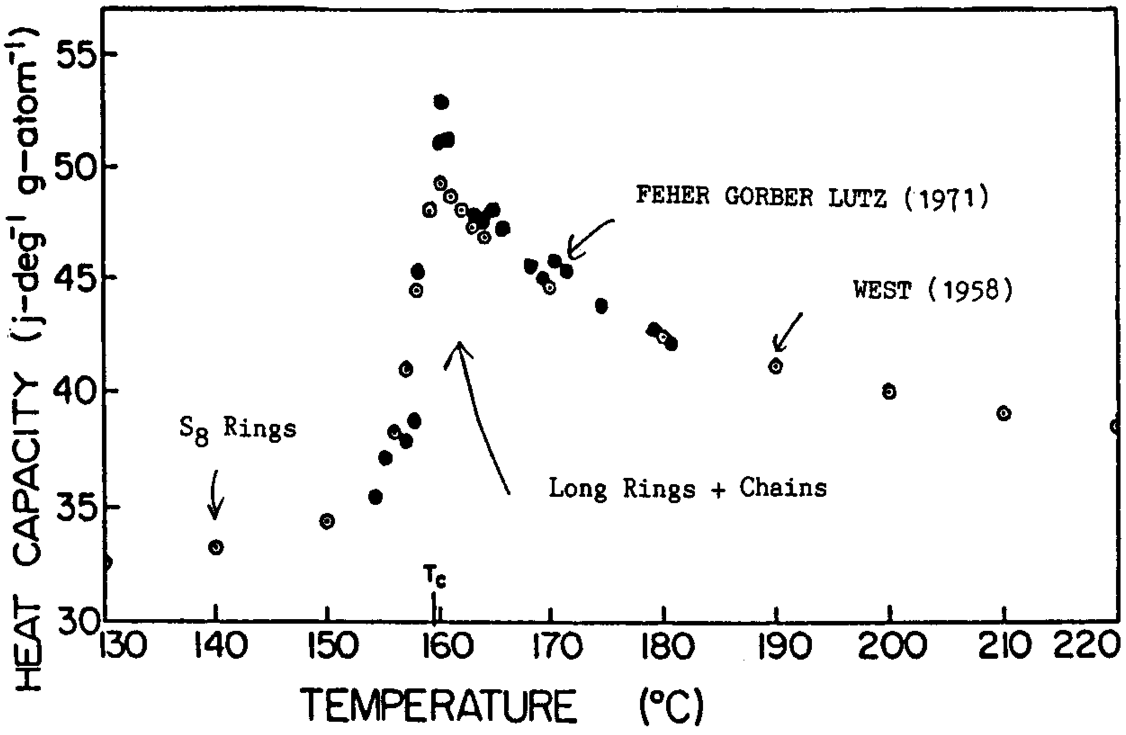

Fig. 2 Polymerization of Sulfur

with the Ising model having $1+\frac{1}{2}\alpha^2$ replaced by $\Sigma_n \alpha^{2n}/(2n)! = \mathrm{ch}\alpha$ and $v = \mathrm{th}\beta$. By a further simple manipulation we were also to transform the integration variables α and u to the Ising variables $s_i(\vec{x}) = \pm 1$ on links and found the representation[5)]

$$Z = 2^{-DN} \sum_{\{s_i(\vec{x})=\pm 1\}} \prod_{\vec{x}} [1 - vD + \tfrac{1}{2} vs^2] \tag{3}$$

where

$$s(\vec{x}) \equiv \sum_i [s_i(x) + s_i(x-i)] \tag{4}$$

is the sum of the Ising values over all links around each site.

The Ising model itself can also be brought[6)] to $s_i(\vec{x})$ variables. In this case the integrand in (3) reads

$$\begin{aligned} &\prod_{\vec{x}} [1 - vD + \tfrac{1}{2}v\, s^2 + v^2(\tfrac{1}{24}\, s^4 - \tfrac{2}{3}\, s^2 + 1)]; \qquad D=2 \\ &\prod_{\vec{x}} [1 - vD + \tfrac{1}{2}v\, s^2 + v^2(\tfrac{1}{24} s^4 - \tfrac{7}{6}\, s^2 + 3) \\ &\qquad + v^3(\tfrac{1}{720} s^6 - \tfrac{5}{72}\, s^4 + \tfrac{34}{45}\, s^2 - 1)]; \; D=3 \end{aligned} \tag{5}$$

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Using this latter result we were able to define a model whose partition function interpolates smoothly between the Ising model and an ensemble of self-avoiding random loops. A detailed study of this model by analytic[5)] and Monte Carlo methods in two[6)] as well as three dimensions[7)] gave convincing evidence that self-avoiding random loops are in the same universality class as Ising loops.

The three-dimensional Monte Carlo data are shown in Fig. 3 and

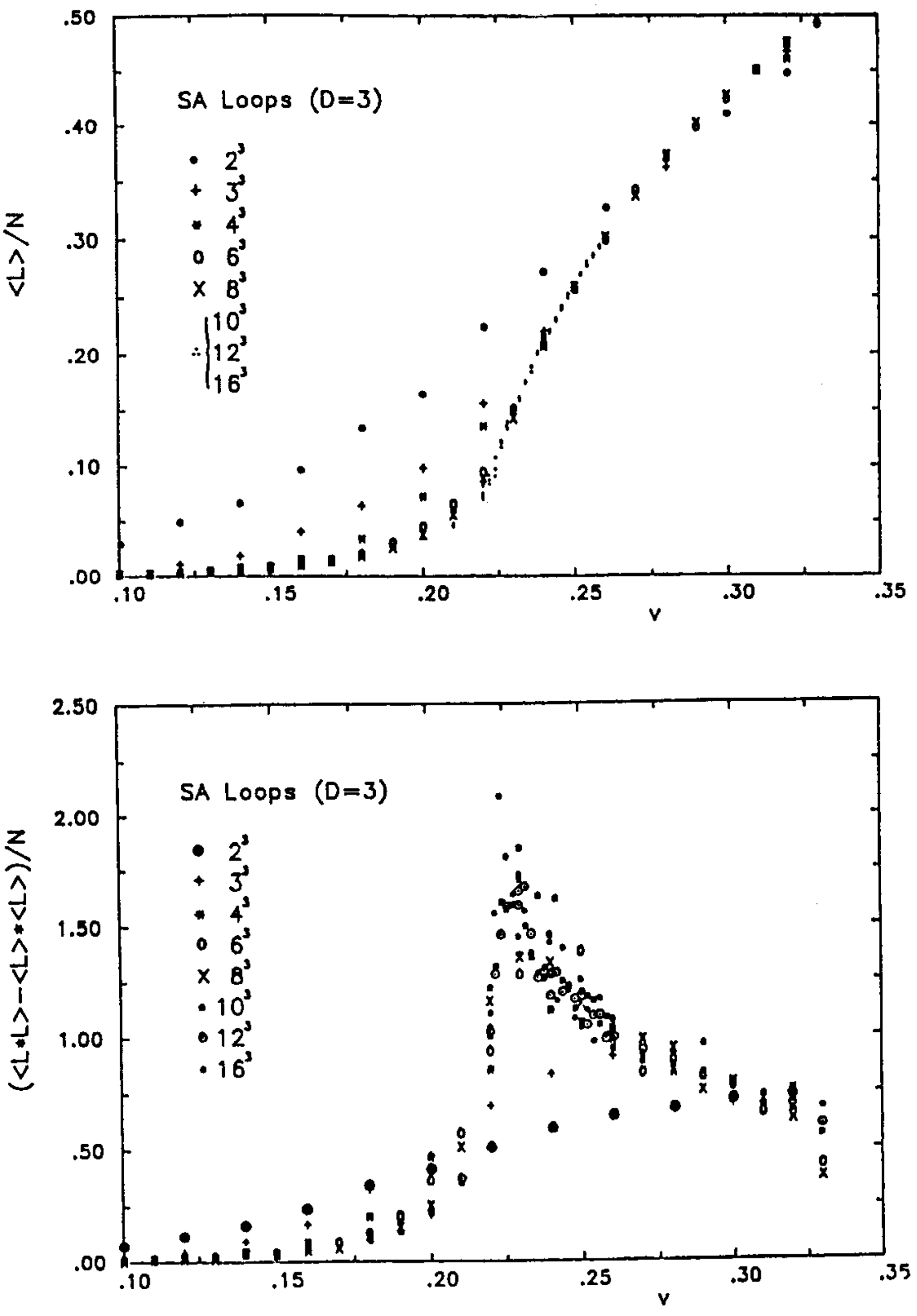

Fig. 3 Mean length and length fluctuations in ensemble of self-avoiding random lines: The peak in the latter curve agrees precisely with the peak in Fig. 2.

the specific heat is seen to have the same shape as the experimental one in Fig. 2.

Let us now turn to the second topic, i.e. self-avoiding random surfaces. Random surfaces have recently gained increasing attention for several reasons. Most fundamentally, they are important for understanding the forces between the constituents of matter (quarks). These forces are due to color electric flux strings which, as a function of time, sweep out surfaces in space time. As long as the vacuum contains only a few smooth surfaces, the quarks can never come apart (confinement). The question of quark confinement is therefore intimately related to the question of the proliferation of surfaces in the vacuum (via entropy energy arguments).

But random surfaces have many more applications, some of which are of economic interest. Amphiphilic soap molecules brought into a system of oil and water form a layer at the oil-water interface (see Fig. 4). Under convenient circumstances the interfacial energy and the curvature energy become so small(8) that droplets of oil begin to invade into the water side and vice versa (see Fig. 5) leading to the formation of microemulsions (see Fig. 6)(9). Microemulsions will be an important tool of extracting the residual oil of depleted oil fields (tertiary oil recovery). Notice that after depletion of a well there is about twice as much oil left as has already been extracted.

There are further applications in other industrial sectors of which I just mention octane improvement, pollution abatement, chemical processing, lubricants, surface coatings, pesticides, cosmetics, biomembranes, and medicine. It is therefore worthwhile studying systems of random surfaces.

It is obvious that the surfaces consisting of soap molecules are self-avoiding. As a first step towards a microscopic theory, we were therefore led to construct a lattice model of self-avoiding surfaces (on a simple cubic lattice). This can be done in complete analogy to the self-avoiding random lines(10). The partition function reads

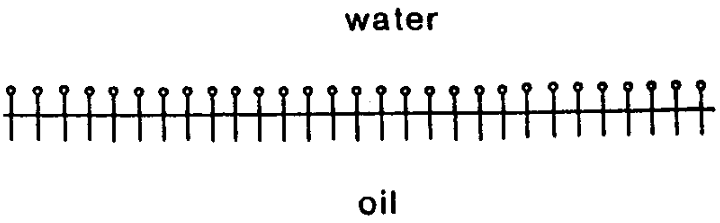

Fig. 4 Amphiphilic molecules at the interface water-oil

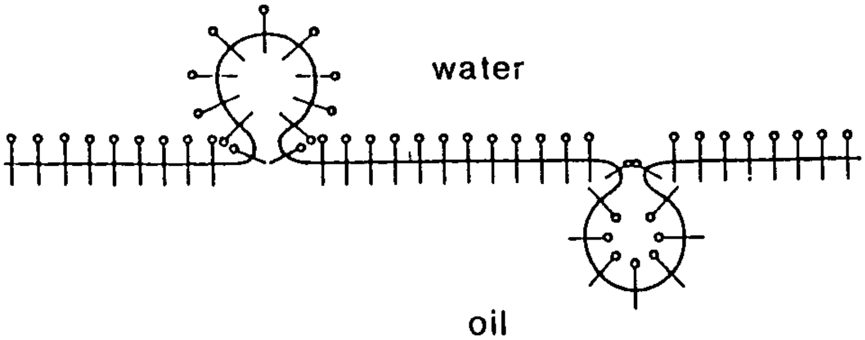

Fig. 5 The nucleation of microemulsion

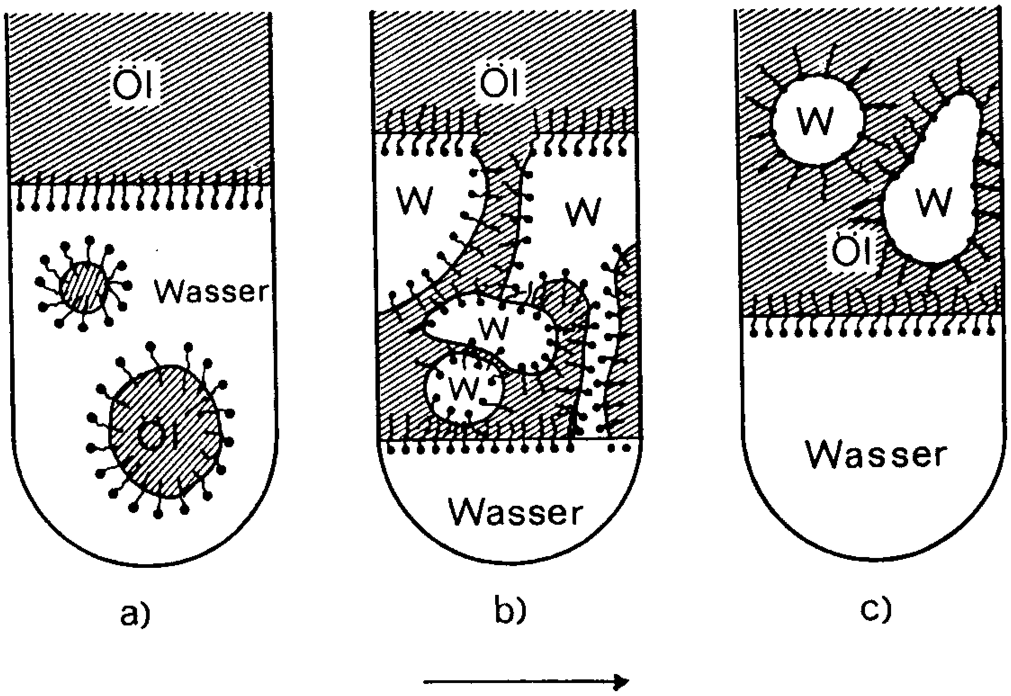

Fig. 6 The sponge-like surface structures in a microemulsion

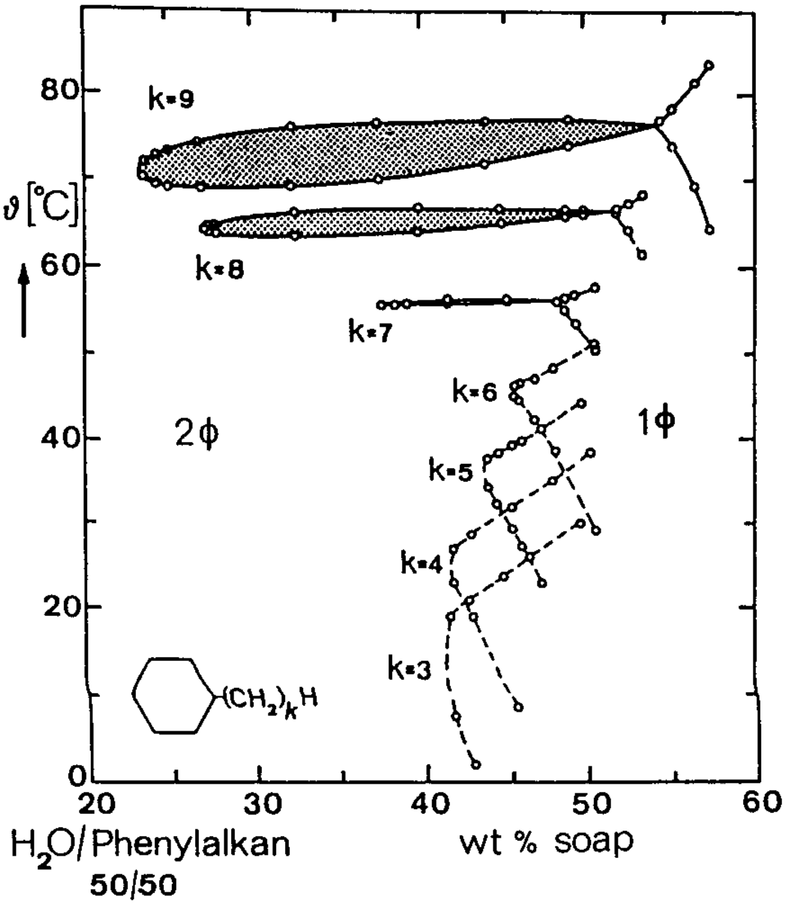

Fig. 7 The phase diagram of a mixture with equal amounts of water and oil as a function of soap concentration (x-axis) and temperature (in °C). The solid curve is from mean-field ϕ^6-theory.

$$Z = \prod_{\vec{x}} \left[\int_{-\pi}^{\pi} \frac{d\theta(\vec{x})}{2\pi} \{ 1 + u_i^{*2}(\vec{x}) \} \right] \prod_{\vec{x}, i<j} [1 + v \, u_i(\vec{x}) \, u_j(\vec{x}+\vec{i}) \, u_i(\vec{x}+\vec{j}) \, u_j(\vec{x})], \qquad (6)$$

where $u_i(\vec{x})$ are pure phase variables $\exp[i\theta_i(\vec{x})]$ on links $\vec{i}$ and $v = \exp(-\epsilon/T)$ the Boltzmann factor for an elementary surface element. The formula is again easy to interpret. The right-hand product distributes all possible surface elements over the plaquettes $i < j$ of the lattice (at most one on each plaquette) whereupon the integration either annihilates the element (1) or welds two adjacent ones together (u_i^{*2}). The model is now closely related to the Ising like lattice gauge theory which differs from it by having $1 + u_i^{*2}$ replaced by the infinite series $1 + u_i^{*2} + u_i^{*4} + \ldots$ and is in turn dual to the D=3 Ising model itself.

The model can again be transformed to real variables on links $\alpha_i(\vec{x})$ and $u_i(\vec{x})$, and to the Ising variables on plaquettes $s_{ij}(\vec{x})$. For further details see the original paper.10)

In order to simulate microemulsions, the model requires the inclusion of curvature energies.11) Near the critical regime, this leads to a mean field energy of the type

$$-\beta f = \xi_o^2 (\partial \phi)^2 + a_1\phi + a_2\phi^2 + a_3\phi^3 + a_4 - \frac{3}{2}\phi^4 + \phi^6 \qquad (7)$$

(after a rescaling of field variables). Such energies have been studied in great detail12) and recently led to a simple explanation of experimental phase diagram (see Fig. 7) as well as interfacial tensions and light scattering data.13)

References

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