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LETTER TO THE EDITOR

Second-order phase transition in a system with weak asymmetry coupling to a non-ordering parameter

Ya'akov Achiam

Department of Mathematical Physics, The University of Birmingham, PO Box 363, Birmingham B15 2TT, UK

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Abstract. Renormalisation group methods are used to analyse a phenomenological model of fluids with a coupling to a non-ordering parameter y, which is asymmetric with respect to the order parameter. The correlation function of y is studied above and below T_c. The critical isochore is found to have a singular term of the order $|T-T_c|^{3\beta+\delta}$, in addition to a shift in the critical field and the critical order parameter.

In every real system undergoing a phase transition there exists a coupling of the order parameter (S) to other degrees of freedom which would not be critical by themselves. The critical behaviour of these non-ordering parameters (NP) is a source of information about the behaviour of S, the critical indices and the interactions between S and NP. However, extraction of such information from an experiment can be done only after pre-study of the appropriate models. In this letter we present a model for the coupling between the polarisation of the molecules and S, in binary mixtures and liquid–gas transitions. These systems, having polar and non-polar components, are the subject of current research (Hocken *et al* 1976, Givon *et al* 1974). We hope that the result we obtain can help in the analysis of experiments which are carried out in similar systems.

We assume that the systems we are interested in can be represented by a lattice-gas model. One can define a polarisation field y_i and a projection operator $(1+S_i)/2$ which describes the occupation of the i site. The additional energy due to the polarisation can be written approximately as $\frac{1}{4}\Sigma_{i,j}(S_i+1)y_i(S_j+1)y_j$. The transformation to continuum fields will cause the appearance of an asymmetric interaction term of the form $\int_x S(x)y^2(x)\,d^dx$ in the Hamiltonian $\mathscr{H}$. This term is added to the usual Landau–Ginzburg Hamiltonian (Wilson and Kogut 1974). A similar term was already included in $\mathscr{H}$ by Siggia *et al* (1976) who presented a model of binary mixtures and liquid–gas transitions in which y is the transverse vector field corresponding to the momentum density.

The Hamiltonian appearing in the partition function Z which we discuss is

$$-\mathscr{H}=\int_\Omega d^dx\ (\tfrac{1}{2}(\nabla S)^2+\tfrac{1}{2}rS^2+uS^4-hS+\tfrac{1}{2}y^2+vy^2S).$$

The first four terms are the Landau–Ginzburg–Wilson Hamiltonian of a $d(=4-\epsilon)$ dimension system with a volume Ω. r and u are the usual parameters (Wilson and Kogut 1974) and h is an external field. The last two terms describe the bare Gaussian contribution of the NP, and the interaction term which was already discussed. The renormalisation group (RG) analysis of $\mathscr{H}$ shows that the first five terms are the only relevant ones. The interaction term is irrelevant (in the RG sense). Any other term, not included in $\mathscr{H}$, is more irrelevant.

The first physical quantities we are interested in are the NP susceptibility, χ_y, and the y–y correlation function at momentum q, Γ_y^q. To find χ_y, one has to add a NP field term, $E \int y(x)$, to $\mathscr{H}$ and perform $\partial^2 \ln Z/\partial E^2$. y can be shifted and integrated out by Gaussian integration. The resultant parameters in the effective Hamiltonian depend on E^2. Thus the critical temperature, field and $\langle S\rangle$ will be shifted proportional to E^2. We have here an example of a system showing $\mathrm{d}T_c(E)/\mathrm{d}E = 0$ at $E = 0$. From general arguments (Fisher 1968, Wegner 1975, Achiam and Imry 1975) one can expect a $|t|^{1-\alpha}$ singularity, where $t = T - T_c$ and α is the specific heat index. In this particular coupling of NP a stronger singularity, $|t|^{\beta}$, appears below T_c (β is the coexistence curve index).

The technique just described cannot work for the calculation of Γ_y^q. This can be evaluated by using a standard RG technique like the matching procedure which will be described briefly at the end of this letter. This analysis to order $v^3 \sim O(\epsilon^{3/2})$ (one loop order) reveals that Γ_y^q is independent of q. As a result, the scaling law relating the singular terms of $\Gamma_y^q(T = T_c)$ and $\Gamma_y^{q=0}(T - T_c)$ is not satisfied. We note that in other coupling of NP (Achiam and Imry 1975, Achiam 1977) such a scaling law is usually found.

Explicitly, we found:

(a) $T > T_c$: $\chi_y \sim 1 + D^+ t^{1-\alpha}$;
(b) $T < T_c$: $\chi_y \sim 1 + D_1^-(-t)^{1-\alpha} - D_2^-(-t)^{\beta} - D_3^-(-t)^{2\beta}$, where $\alpha = 2 - d\nu = \epsilon/6 + O(\epsilon^2)$ and $\beta = \frac{1}{2} - \epsilon/6 + O(\epsilon^2)$.

The ratios of the amplitudes are: $D^+/D_1^- = A^+/A^-$ where $A^{\pm}$ are the amplitudes of the specific heat $C = A^{\pm}|t|^{-\alpha}$, $t \to \pm 0$, $(D_2^-)^2 A^-/D_1^- = (1-\alpha)2^{2\beta}(8u^*)$ where u^* is the fixed point of u, $u^* = \epsilon/(36K_4) + O(\epsilon^2)$.

Our next problem is to find how the asymmetric coupling of the NP affects the critical behaviour of S. Again, one can perform a Gaussian integration of y in Z. This procedure creates an effective Hamiltonian $\mathscr{H}_{\text{eff}}$. Its parameters $-H$, R and W, the coefficients of $\sigma = S - \langle S\rangle$, σ^2 and σ^3 respectively, are related to the original ones as follows: $R = \tilde{r} - 2\tilde{v}^2$, $W = 4um + 4/3\tilde{v}^3$ and $H = \tilde{h} - \tilde{v}$, where $m = \langle S\rangle$, $\tilde{v} = v/(1 + 2vm)$, $\tilde{r} = r + 12um^2$ and $\tilde{h} = h - rm - 4um^3$. $\mathscr{H}_{\text{eff}}$ has the same form as the 'ideal' ($v = 0$) Ising Hamiltonian in the presence of a magnetic field (Brézin *et al* 1973, Rudnick and Nelson 1976, Achiam and Kosterlitz 1977). As a consequence, the critical behaviour of S remains 'ideal' except for the following shifts in the critical values of the thermodynamic quantities:

$$m_c = -v^3/(3u^*) \qquad \Delta T_c = 2v^2 \qquad h_c = v.$$

The combination $\Delta = \Delta T_c h_c/m_c$ has to $O(\epsilon)$ a universal value, $\Delta = -\epsilon/(6K_4)$. The parameters of $\mathscr{H}$ (or $\mathscr{H}_{\text{eff}}$) enter into the thermodynamic functions (e.g. equation of state) via a combination called scaling fields. These are quantities which scale with a pure exponent under RG. If the combinations of v with the other parameters of $\mathscr{H}$, as found in the parameters of $\mathscr{H}_{\text{eff}}$, are the same as those entering into the scaling fields, the shifts in h_c, ΔT_c and m_c, which were mentioned above, would be the only effects of the NP. However, that does not have to be the case, and indeed it is not. Then, if one were to integrate y from Z at the l stage of RG, corrections to the new effective parameters would be necessary in order to have the scaling fields. These corrections are equivalent to singular contributions to the critical values of the thermodynamic quantities. It is not difficult to see that in our approximations the only singularity can be found in h_c. The correction to the scaling fields can enter only through v which does not appear in the ideal Hamiltonian. The m_c is already $O(v^3)$. Correction to it will be of higher order. But in h_c which is $O(v)$, corrections may be found. Indeed, the RG calculations of the equation of state show

$$h_c = v_0 - [\tfrac{3}{2} - 4(1+2K_4/d)]K_4 v_0^3 t^{\phi_h} \qquad \text{where } \phi_h = 3\beta + \delta$$

($\delta = 3 + \epsilon + O(\epsilon^2)$, $K_4 = 1/8\pi^2$). This is a very small singularity which satisfies Griffiths' inequality: $\phi_h \geqslant 2 - (\alpha + \beta)$ (Griffiths 1965). As was already mentioned, $m_c(t)$ is a straight line. Mermin and Rehr (1971, and references therein) argued that if the tangent to the coexistence curve at the critical point of a liquid–gas transition is not parallel to the temperature or field axes, the singularity of $m_c(t)$ is at least $|t|^{1-\alpha}$. This singularity has not been found yet experimentally (Levelt Sengers and Chen 1972). Our model does not satisfy the preliminary conditions on the tangent. Hence the missing singularity of $m_c(t)$ is not a surprise. However, it is not impossible that analysis to high orders will reveal such a singularity.

To end this letter, we shall discuss briefly the RG calculations which led us to the above results. The recursion relations (RR) which the parameters of $\mathscr{H}_l$ obey are thus of the ideal system (Rudnick and Nelson 1976) to which the contributions of v are added, the RR of v and the scaling of y. The solutions of these RR to order v^3 (one loop expansion) are:

$$\rho_l \equiv \tfrac{1}{2} + v_l m_l = \rho_0 \qquad \text{(fixes the rescaling of } y\text{)}$$

$$v_l + 4K_4 v_l^3 \equiv V_l = V_0 \exp(\lambda_v l) \qquad \lambda_v = -(1-\epsilon/2)$$

$$m_l + K_4 V_l^3/12u^* \equiv M_l = M_0 \exp(\lambda_m l), \qquad \lambda_m = -\lambda_v$$

$$\tilde{r}_l - 12u^* M_l^2 + 6K_4 u^* - K_4 v_l^2/2 \equiv t_l = t_0 \exp(\lambda_t l) \qquad \lambda_t = 2 - \epsilon/3$$

$$\tilde{h}_l + t_l M_l + 4uM_l^3 - 6K_4 u^* M_l - K_4/d v_l + (4 + 8K_4/d)K_4 v_l^3 + \tfrac{1}{24} v_l^5/u^*$$

$$\equiv H_l = H_0 \exp(\lambda_h l) \qquad \lambda_h = \beta\delta/\nu.$$

Two remarks should be mentioned at this point.

(i) These are the solutions which are linear in r_l. Although we should iterate them up to $r_l \sim O(1)$, the non-linearity in r only causes slight changes in the definition of the scaling field which cancelled in the calculation of thermodynamic quantities (see discussion by Achiam and Kosterlitz 1977).

(ii) By comparing the results for m_c, h_c and ΔT from the scaling fields and from $\mathscr{H}_{\text{eff}}$, one can find disagreement by a factor K_4/d. This is due to the particular shape of the Brillouin zone we work with, and is not significant.

We used the 'matching procedure' in the framework of RG. (More details concerning this technique can be found in Achiam and Kosterlitz (1977), Rudnick and Nelson (1976) and references therein.) Starting with $\mathscr{H}$ one may generate a sequence of $\mathscr{H}_l$, similar to $\mathscr{H}$, by integrating out σ_q and y_q with $1 > q > e^{-l}$ which appear in Z. Then the q, σ_q and y_q are rescaled: $q_l = e^l q$, $\sigma_q = \zeta(l)\sigma^l_{q_l}$, $y_q = c(l) y^l_{q_l}$ such as to keep $\mathscr{H}_l$ in similar form to $\mathscr{H}$. Γ_y and $\Gamma_y(l)$ are calculated in $\mathscr{H}$ and $\mathscr{H}_l$, respectively. They are related via $\Gamma_y = c^2(l)\exp(-dl)\Gamma y(l)$. We calculated $\chi_y(L)$ when $\tilde{r}(L) + q_L^2 \sim 1$. This condition (Nelson 1976) serves as an infrared cut-off, and enables us to calculate $\chi_y(L)$

by the Dyson equation. The leading singularity in $c\exp(-dl/2)$ is $\exp(-2\beta l/\nu)$. However, this singularity cancelled out in the calculation of Γ_y. Only the $|t|^{1-\alpha}$ singularity is found, resulting from an energy-like term.

From the condition $\langle\sigma\rangle = 0$ evaluated using perturbation expansion at the L stage of RG we found $m_L = f(H_L)$. Using the RR we obtained the equation of state.

We conclude with a remark on the role of other transients in the above model. All the RG calculations were performed at the fixed point of $u = u^*$. If the initial u is not at its fixed-point value, we expect very slow transients, typical of the crossover between the Gaussian and Ising fixed points. The above treatment can be generalised easily to this case in a similar way to that done by Rudnick and Nelson (1976). It results in more complicated scale functions. The second transient is the one from the term σ^5. We assume an ideal symmetric model. Hence such a parameter is of order v^5, and can be neglected. However, one has to remember that it has a transient which decays similarly to $v(l)$. A term σ^5 was found in a liquid–gas transition by Hubbard and Schofield (1972). It is reasonable to suppose that it creates corrections to h_c and m_c similar to those found here, but such an analysis is beyond the scope of the present work.

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References

Achiam Y 1977 *J. Phys. C: Solid St. Phys.* **10** 1491
Achiam Y and Imry Y 1975 *Phys. Rev.* B **12** 2768
Achiam Y and Kosterlitz J M 1977 *J. Phys. C: Solid St. Phys.* **10** 4559
Brézin E, Wallace D J and Wilson K G 1973 *Phys. Rev.* B **7** 232
Fisher M E 1968 *Phys. Rev.* **176** 257
Givon M, Pelah I and Efron U 1974 *Phys. Lett.* **48A** 1
Griffiths R B 1965 *J. Chem. Phys.* **43** 1958
Hocken R, Horowitz M A and Greer S C 1976 *Phys. Rev. Lett.* **37** 964
Hubbard J and Schofield P 1972 *Phys. Lett.* **40A** 245
Levelt Sengers J M H and Chen W T 1972 *J. Chem. Phys.* **56** 595
Mermin N D and Rehr J J 1971 *Phys. Rev. Lett.* **26** 1155
Nelson D R 1976 *Phys. Rev.* B **14** 1123
Rudnick J and Nelson D R 1976 *Phys. Rev.* B **13** 2208
Siggia E P, Halperin B I and Hohenberg P C 1976 *Phys. Rev.* B **13** 2110
Wegner F J 1975 *J. Phys. A: Math. Gen.* **8** 710
Wilson K G and Kogut J 1974 *Phys. Rep.* **12** 75