Competing Interactions, the Renormalization Group, and the Isotropic-Nematic Phase Transition

Daniel G. Barci[1,3] and Daniel A. Stariolo[2,3]

[1]*Departamento de Física Teórica, Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier 524, 20550-013, Rio de Janeiro, RJ, Brazil*

[2]*Departamento de Física, Universidade Federal do Rio Grande do Sul, CP 15051, 91501-970, Porto Alegre, Brazil*

[3]*The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy*

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We discuss 2D systems with Ising symmetry and competing interactions at different scales. In the framework of the renormalization group, we study the effect of relevant quartic interactions. In addition to the usual constant interaction term, we analyze the effect of quadrupole interactions in the self-consistent Hartree approximation. We show that in the case of a repulsive quadrupole interaction, there is a first-order phase transition to a stripe phase in agreement with the well-known Brazovskii result. However, in the case of attractive quadrupole interactions there is an isotropic-nematic second-order transition with higher critical temperature.

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The interest in phases with complex translational and/or orientational order has been growing in the condensed matter community in recent years. Systems with very different microscopic origin present phase transitions from disorder isotropic, homogeneous phases to anisotropic and/or inhomogeneous ones. The physical origin of this behavior is in many cases associated with the competition between short-ranged attractive and long-ranged repulsive interactions [1]. The attractive part tends to form ordered phases or condensates, or in the case of conserved order parameter, tends to produce phase separation. However, a long-ranged repulsion frustrates this tendency, favoring the emergence of complex phases that break translational and/or rotational symmetry. Examples of these systems go from highly correlated quantum systems like quantum Hall samples [2,3] and high-T_c superconductors [4] to classical systems like ferromagnetic films [5,6], diblock copolymers [7], and liquid crystals [8,9], to name but a few. All these systems have a special regime where physical properties are dominated by an extended region in momentum space with large degeneracy. For instance, in Fermi liquids this degeneracy is related to the existence of a Fermi surface at low temperatures. In classical systems, the competing interactions lead to a shift of the dominant wave vector in the structure factor to a nonzero value. In nearly isotropic systems, the low energy degrees of freedom are kinematically constrained to a thin spherical shell of radius k_0 determined by interactions. Examples of scalar and vector order parameters behaving this way were studied by Brazovskii in a seminal work [10]. He showed that in systems with a spectrum of fluctuations dominated by a nonzero wave vector, there is a first-order phase transition at a finite temperature form an isotropic to a stripe phase, induced by field fluctuations. His prediction was experimentally confirmed in the microphase separation transition in diblock copolymers [11]. It is also observed in Monte Carlo simulations of ultrathin magnetic films with perpendicular anisotropy [12] and in the Coulomb frustrated ferromagnet [13], where the first-order transition is clearly seen. However, theoretical and numerical work on ferromagnetic films [5,14] and the classic KTHNY theory of two dimensional melting [15] predict a more complex phase diagram. For instance, it could be possible to melt the stripes into a nematic phase, where the translational order is lost, but orientational order remains.

With this motivation we review in this Letter the effective low energy theory for systems with competing interactions under the perspective of the renormalization group (RG) [16]. The presence of a new scale k_0 with a large momentum space allowed for fluctuations completely changes the properties of the Gaussian fixed point. We found that, upon expanding the angular momentum content of the interaction, the $d = 2$ system is characterized by an infinite number of relevant quartic coupling constants. This result resembles the Fermi liquid theory where there is an infinite number of marginal Landau parameters controlling the fixed point [17]. In particular, we found that the first nontrivial coupling after the usual local ϕ^4 theory represents an interaction between local quadrupole moments. If this interaction is repulsive, the Brazovskii analysis remains the correct one, predicting a first-order transition to an inhomogeneous state. However, if this interaction is attractive, there is a new instability describing a second-order isotropic-nematic phase transition with critical temperature higher than the melting transition of the Brazovskii model. We have characterized this $d = 2$ nematic critical point in the self-consistent Hartree approximation. We have computed the critical temperature T_c as well as the critical exponents $\beta = 1/2$, $\gamma = 1$. The conditions for the existence of the nematic phase and its critical properties are the main results of this Letter. In the rest of the Letter we sketch the analysis leading to these results.

In general, the low temperature physics of $2d$ models with competing interactions and Ising symmetry is well described by a coarse-grained Hamiltonian of the type

$$H_0 = \int_\Lambda \frac{d^2k}{(2\pi)^2}\,\phi(\vec{k})\left(r_0 + \frac{1}{m}(k-k_0)^2 + \cdots\right)\phi(-\vec{k}), \tag{1}$$

where $r_0(T) \sim (T - T_c)$, $k = |\vec{k}|$, and $k_0 = |\vec{k}_0|$ is a constant given by the nature of the competing interactions. $\int_\Lambda d^2k \equiv \int_0^{2\pi} d\theta \int_{k_0-\Lambda}^{k_0+\Lambda} dkk$ and $\Lambda \sim \sqrt{mr_0}$ is a cutoff where the expansion of the free energy up to quadratic order in the momentum makes sense. The "mass" m measures the curvature of the dispersion relation around the minimum k_0 and the "$\cdots$" in Eq. (1) means higher order terms in $(k - k_0)$. The structure factor has a maximum at $k = k_0$ with a correlation length $\xi \sim 1/\sqrt{mr_0}$. Therefore, near criticality ($r_0 \to 0$) the physics is dominated by an annulus in momentum space with momenta $k \sim k_0$ and width 2Λ. This situation is quite similar with fermionic systems at low temperature, where the role of k_0 is the Fermi momentum, and the reduction of phase space to a spherical shell centered at the Fermi momentum is ruled by the Pauli exclusion principle. In our case of interest, the microscopic physics is very different, but the effects of kinematical constraints on momentum space are equivalent.

We would like to determine what kind of interaction terms are relevant to study the low energy physics of a system given by the Hamiltonian of Eq. (1). The method is similar to the RG for Fermi liquids developed in Ref. [18] and already applied to the Brazovskii model in Ref. [19] to study the first-order transition to the stripe phase. The standard procedure is to identify a scale transformation that leaves the Gaussian theory invariant, and then study the relevance of interactions in the scaling limit very near the circle $k = k_0$. With this aim, as usual, we define a small radial wave vector $q = k - k_0$, we reduce the cutoff to Λ/s, with $s > 1$, and integrate over rapid modes $\Lambda/s < |q| < \Lambda$, then we rescale the fields and wave vectors to reestablish the same scale and compare the couplings. First, note that the kinetic term in Eq. (1) is invariant under the rescalings

$$\Lambda' = \Lambda/s, \tag{2}$$

$$q' = sq, \tag{3}$$

$$\phi'(q') = s^{-3/2}\phi(q'/s). \tag{4}$$

Some important comments are in order. These transformations are independent of the dimension of the momentum space. This result is very different for systems without competing interactions where $k_0 = 0$. In this case, the fields would scale as $\phi'(q') = s^{-(d+2)/2}\phi(q'/s)$, where d is the spatial dimension of the system. This fact leads to a completely different analysis in the case of competing interactions. In fact, the usual concepts of upper and lower critical dimensions will change in our case, due essentially to the degeneracy of the lowest energy manifold. With this scaling in mind we immediately conclude that the term $r_0|\phi|^2$ in Eq. (1) is relevant as it should be, as this term controls criticality. Let us now analyze a generic quartic interaction (we do not analyze cubic terms in this article since we are interested in systems with Ising symmetry $\phi \to -\phi$):

$$H_{\rm int} = \int_\Lambda \frac{d^2k_1}{(2\pi)^2}\frac{d^2k_2}{(2\pi)^2}\frac{d^2k_3}{(2\pi)^2}\frac{d^2k_4}{(2\pi)^2}u(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\phi(\vec{k}_1) \times \phi(\vec{k}_2)\phi(\vec{k}_3)\phi(\vec{k}_4)\delta(\vec{k}_1+\vec{k}_2+\vec{k}_3+\vec{k}_4). \tag{5}$$

Changing variables $q_i = k_i - k_{0i}$, with $i = 1, \ldots, 4$, and rescaling the momenta and fields following Eqs. (2)–(4), we obtain at "tree level" $u'(q_1', q_2', q_3', q_4') = s^3 u(q_1'/s, q_2'/s, q_3'/s, q_4'/s)$ [20]. We immediately see that the constant term is relevant. Therefore, at this level of approximation it is enough to keep the quartic term replacing $q_i = 0$ in the expression for $u(q_i)$. It is important to note a difference with the case $k_0 = 0$; even though the coupling u is a constant, in the sense that it does not depend on q, it still depends on the angles θ_i of each $\vec{k}_{0i}$, and then $u \equiv u(\theta_1, \theta_2, \theta_3, \theta_4)$. However, these angles are strongly constrained by kinematics. Momentum conservation allows us to eliminate one of them in terms of the other three. Furthermore, as the momenta are constrained to move in a very narrow circular region of radius k_0 and width Λ, we can fix only two of them and the other two are automatically slaved. Finally, since the system is rotational invariant, the couplings can only depend on the difference between these two angles, $u(\theta_1, \theta_2, \theta_1 + \pi, \theta_2 + \pi) = u(\theta_1 - \theta_2) = u(\theta)$. Thus, the quartic interaction is represented, not by few constants, but by a continuous function of an angle. There is still a last constraint, due to the fact that $u(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4)$ in Eq. (5) is invariant under any permutation of the four indexes, implying that $u(\theta) = u(\theta + \pi)$. Therefore, we can expand $u(\theta)$ in a Fourier series, obtaining an infinite set of coupling constants representing angular momentum "channels" of the interaction:

$$u(\theta) = u_0 + u_2\cos(2\theta) + u_4\cos(4\theta) + \cdots. \tag{6}$$

The first term u_0 leads to the usual ϕ^4 theory considered by Brazovskii in his model for the isotropic-smectic transition. In Ref. [19] a detailed RG analysis showed the evolution of the running coupling constants u_0 and r_0 far from criticality, $T \ll T_c$. This analysis is justified because it is in this region that the fluctuation induced first-order transition occurs. In this Letter we are interested in another regime, $T \sim T_c$, where the whole set of couplings

$\{u_0, u_2, u_4, \ldots\}$ has to be considered, in principle, at the same level. A detailed analysis of the RG flow will be presented elsewhere [21].

For simplicity, let us consider the effect of the first two terms. A convenient way of representing the Hamiltonian in terms of u_0 and u_2 in real space is

$$H_{\rm int} = \int d^2x\{u_0\phi^4(\vec{x}) + u_2\,{\rm tr}\hat{Q}^2\}, \tag{7}$$

where

$$\hat{Q}_{ij}(\vec{x}) = \phi(\vec{x})\left(\nabla_i\nabla_j - \frac{1}{2}\nabla^2\delta_{ij}\right)\phi(\vec{x}) \tag{8}$$

can be easily recognized as the quadrupole moment of the density ϕ^2 [22].

$\hat{Q}_{ij}$ is a traceless symmetric tensor, being a natural local order parameter for a phase with orientational order. In fact, a phase with $\langle\phi(\vec{x})\rangle = 0$ and $\tilde{Q}_{ij} \equiv \int dx \langle\hat{Q}_{ij}(\vec{x})\rangle \neq 0$ is a homogeneous phase, with orientational order with the nematic symmetry $\theta \to \theta + \pi$. In the following, we will show that under certain conditions this is the ordered phase produced at the onset of the instability $r_0 \sim 0$.

To study this phase transition, we make a self-consistent Hartree approximation and analyze the Hamiltonian Eq. (7) in the same lines of Brazovskii's work [10]. This approximation is exact in an $O(N)$ model in the limit $N \to \infty$. In our case, it will present $1/N$ corrections. In this analysis, we should also consider corrections of the type $\gamma\,{\rm tr}\hat{Q}^4$ with $\gamma > 0$. Although this term does not enter the critical properties of the system at this level of approximation, it will be important to stabilize the low temperature phase.

As usual, we replace in Eq. (7) $\phi^4 \to \phi^2\langle\phi^2\rangle$ and ${\rm tr}\hat{Q}^2 \to {\rm tr}\{\phi(\nabla_i\nabla_j - \frac{1}{2}\nabla^2\delta_{ij})\phi\}\langle\hat{Q}_{ij}(\vec{x})\rangle$, where the mean values will be determined self-consistently. With this procedure we obtain a quadratic Hamiltonian in the Hartree approximation given in momentum space by

$$H_{\rm Hartree} = \frac{1}{2}\int\frac{d^2k}{(2\pi)^2}\phi(\vec{k})(\beta^{-1}C^{-1}(\vec{k}))\phi(-\vec{k}), \tag{9}$$

where the static structure factor $C(\vec{k})$ is now given by

$$C(\vec{k}) = \frac{T}{r + \frac{1}{m}(k-k_0)^2 - \alpha k^2\cos(2\theta)(u_2 + \gamma\alpha^2)}, \tag{10}$$

and

$$r = r_0 + u_0\int\frac{d^2k}{(2\pi)^2}C(\vec{k}), \tag{11}$$

where we have chosen $\tilde{Q}_{ij} = \alpha(\hat{n}_i\hat{n}_j - \frac{1}{2}\delta_{i,j})$ and we have absorbed unimportant numerical factors in the definition of u_0. θ is the angle subtended by $\vec{k}$ with the director $\hat{n}$. Note that the new quartic term explicitly introduces an anisotropy in the structure factor of Eq. (10). The coupling has exactly the form of the second term in Eq. (6), as it should be. This new term is also responsible for a shift in the value of the dominant wave vector. From the definition of the nematic order parameter, Eq. (8), we find that the amplitude of $\tilde{Q}_{ij}$ is given by

$$\alpha = -\frac{1}{2}\int\frac{d^2k}{(2\pi)^2}k^2\cos(2\theta)C(\vec{k}) \tag{12}$$

which, together with (10) and (11), completes a set of equations to be solved self-consistently.

After the exact integration over the angles, we have integrated the radial variable k in the limit where the correlation length $\xi \sim 1/(\sqrt{mr})$ is much larger than the typical wavelength of the system $1/k_0$. It can also easily be checked that $\alpha = 0$ is always a solution of Eq. (12), and we expect that at high temperatures this is the only possible solution at finite r. Therefore, upon the k integrations at leading order in $\sqrt{mr}/k_0$, the result can be expanded in powers of α^2/r. It is convenient to write the equations in terms of the adimensional parameters $r \to rT$, $k_0 \to k_0\sqrt{mT}$, and $r_0 \to \tau = c(1 - T_c/T)$, obtaining at leading order in (α^2/r)

$$r = \tau + u_0k_0m\frac{1}{\sqrt{r}} + O\left(\frac{\alpha^2}{r}\right) \tag{13}$$

and

$$\alpha^2\left\{a_1(r,T) + a_2(r,T)\frac{\alpha^2}{r} + O\left[\left(\frac{\alpha^2}{r}\right)^2\right]\right\} = 0, \tag{14}$$

where $a_1(r,T) = u_2(8 + u_2k_0^5m^3T^2/2r^{3/2})$ and $a_2(r,T) = 8r\gamma + k_0^5m^3u_2(\gamma + \frac{15}{64}m^2k_0^4u_2/r^2)/\sqrt{r}$.

From this result, it is clear that if $u_2 > 0$, corresponding to repulsive quadrupolar interaction, $a_1(r,T) > 0$ and $a_2(r,T) > 0$ for all r and T. Therefore, in this case, the only possible solution is $\alpha = 0$. The model then reduces to that of Brazovskii, and a careful study of Eq. (13) follows the same lines of Ref. [10]. In this case nothing happens at $T = T_c$. The system shows a first-order phase transition to a stripe phase, with a melting temperature $T_m \sim T_c/(1 + r_c) < T_c$, where $r_c \equiv r(\tau = 0) = (u_0k_0m)^{2/3}$. However, in the case of attractive quadrupole interactions, $u_2 < 0$, Eqs. (13) and (14) have nontrivial solutions. For high temperatures $T > T_c$ the only possible solution is $\alpha = 0$, as anticipated. This represents a high temperature disordered homogeneous and isotropic phase. On the other hand, if $T < T_c$, a nematic phase emerges continuously with $\alpha \sim |T - T_c|^{1/2}$. From Eqs. (13) and (14) and the condition $a_1(r_c, T_c) = 0$, we can read the critical temperature to be $T_c = 4/(mk_0^2)\sqrt{u_0/u_2}$.

We have also computed the nematic susceptibility, by coupling the system to a small external field conjugate to the nematic order parameter. Considering for simplicity the orientation of the field in the same direction as the order parameter, we find for the nematic susceptibility $\chi_n \sim 1/(T - T_c)$. This confirms the second-order nature of this transition, with critical exponents $\beta = 1/2$ and $\gamma = 1$. One has to bear in mind that these critical exponents will certainly be modified by fluctuations. The reason is that in our Hartree approximation the order parameter Q_{ij} depends on ϕ fluctuations. In other words, it is a Hartree approximation for the order parameter ϕ; however, a mean field one in Q_{ij}. We expect that upon improving this approximation including fluctuations in Q_{ij}, the isotropic-nematic transition should be of the Kosterlitz-Thouless type [21].

In summary, we have analyzed a general model of a scalar field theory with competing interactions in two dimensions. This model is dominated by a small circular shell in momentum space, profoundly modifying the critical properties of the corresponding model without competition ($k_0 = 0$). In particular, we have shown that, in the framework of the renormalization group, the Gaussian fixed point is affected by an infinite set of relevant coupling constants that codify the angular momentum content of a particular microscopic interaction. We have analyzed the simplest model with two coupling constants, corresponding to consider quadrupole moment interactions. We have found that the repulsive case reduces to the well-known Brazovskii model, with a fluctuation induced first-order phase transition to a nonhomogeneous stripe state. However, for attractive quadrupole interactions the phase diagram changes considerably. By applying a self-consistent Hartree approximation in the fields we found a phase transition from a high temperature disordered phase to a nematic phase at lower temperatures. The critical temperature is higher than the melting temperature found by Brazovskii, opening the possibility of having a more complex phase diagram, with an intermediate nematic phase and a possible first-order nematic-stripe phase transition. Whether u_2 is positive or negative in a real system depends on the microscopic interactions. Our results also highlight how to measure nematic order from data for the structure factor and predict the temperature window between T_m and T_c opening the way to look for this phase experimentally, in systems like anisotropic thin film ferromagnets and diblock copolymers, among many others.

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