Quasi-Gaussian approximation and Landau's theory

The universal results that we have derived within the framework of the quasi-Gaussian approximation also follow from Landau's theory of critical phenomena.

Landau's theory is based on general assumptions concerning the properties of systems with short range interactions, of which we have used some to justify the quasi-Gaussian approximation.

Landau's theory takes the form of several regularity conditions of the thermodynamic potential as a function of temperature and local magnetization (more generally of a local order parameter).

(i) The thermodynamic potential $\Gamma(M)$, function of the local magnetization $M(\mathbf{x})$ (generated by an inhomogeneous magnetic field) and generating functional of vertex functions, is expandable in powers of M at $M = 0$.

(ii) We consider only physical systems that in zero field are invariant under space translations. Then, in terms of the Fourier transform of the magnetization field,

$$M(\mathbf{x}) = \int \mathrm{d}^d k \; \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \, \tilde{M}(\mathbf{k}),$$

the thermodynamic potential $\Gamma(M)$ has an expansion of the form

$$\Gamma(M) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \mathrm{d}^d k_1 \ldots \mathrm{d}^d k_n \, \tilde{M}(\mathbf{k}_1) \ldots \tilde{M}(\mathbf{k}_n)$$
$$\times (2\pi)^d \delta^{(d)}\left(\sum_i \mathbf{k}_i\right) \tilde{\Gamma}^{(n)}(\mathbf{k}_1, \ldots, \mathbf{k}_n),$$

where the Dirac $\delta^{(d)}$ functions result from translation invariance, which implies that the sum of Fourier variables must vanish.The vertex functions $\tilde{\Gamma}^{(n)}$, which appear in the expansion, are regular at $\mathbf{k}_i = 0$ (short range interactions).

(iii) The vertex functions $\tilde{\Gamma}^{(n)}$ are regular functions of the temperature for T near T_c, the temperature at which $\tilde{\Gamma}^{(2)}(\mathbf{k}=0)$ vanishes.

Finally, the positivity of $\tilde{\Gamma}^{(4)}(0,0,0,0)$ is a necessary condition for the transition to be second order.

These conditions are motivated by some general assumptions: the effective spins are microscopic averages of weakly coupled variables whose fluctuations can be treated perturbatively.

They rely also on a decoupling of the various scales of physics, and leads to the conclusion that critical phenomena can be described, at leading order, in terms of a finite number of effective macroscopic variables, as in the mean field approximation (MFA).

However, the universal predictions of Landau's theory are in quantitative (sometimes even qualitative) disagreement with experimental results and with results coming from lattice models. An examination of the leading corrections to the Gaussian theory indicates the origin of the difficulty.

Corrections to the quasi-Gaussian approximation

To describe the low temperature phase, it is necessary to go beyond the Gaussian model. But the quasi-Gaussian approximation is justified only if the steepest descent method is justified. Formally, this condition seems to be satisfied if all the coefficients b_{2p} of the expansion of $B(\sigma)$, except the coefficient b_2 of the quadratic term, are in some sense small.

However, it is also necessary that the unavoidable corrections to the leading order result change only the coefficients of the expansion of the thermodynamic potential, without affecting its regularity properties.

This can be verified by calculating the first correction to the second derivative of the thermodynamic potential density, $\mathcal{G}''(0) = \chi^{-1}$, in zero field above T_c (the disordered phase) for $r - r_c \to 0_+$.

The calculation involves two steps: first a determination of the value of r for which $\mathcal{G}''(0)$ vanishes, which yields a non-universal correction to r_c and thus T_c, then a calculation of the leading contribution to $\mathcal{G}''(0)$ for $r \to r_c$.

Perturbative expansion and regularization

To describe physics in the ordered phase below T_c, one needs to perturb the quadratic Hamiltonian by adding higher power terms to the quadratic potential.

Near the transition, the expectation value of the field is small and thus one can make a small field expansion:

$$\mathcal{H}(\sigma) = \mathcal{H}_{\mathrm{G}}(\sigma) + \tfrac{1}{2} b_2 \int \mathrm{d}^d x \, \sigma^2(x) + \frac{b_4}{4!} \int \mathrm{d}^d x \, \sigma^4(x) + \cdots \, .$$

Thermodynamic quantities can then be calculated by expanding in powers of $b_4, b_6 \ldots$.

This involves calculating Gaussian expectation values of $\sigma^2(x)$, $\sigma^4(x)$...

However, the Gaussian two-point function generated by the Hamiltonian $\mathcal{H}_{\mathrm{G}}$ leads to a first non-physical problem: for $d > 1$, too singular, in particular nowhere continuous, fields contribute to the field integral in such a way that correlation functions at coinciding points are not defined.

For example, in all space dimensions $d \geq 2$,

$$\langle \sigma^2(x) \rangle = W^{(2)}(0,0) = \frac{1}{(2\pi)^d} \int \frac{\mathrm{d}^d p}{p^2 + r},$$

diverges for large momenta (reflecting a short distance singularity).

Regularization. The problem of 'UV' divergences, first encountered in QED, is absent in lattice models due to the lattice structure, as well as in other statistical systems due to their intrinsic short distance structure.

It appears here only because one insists on making no reference to a microscopic scale (decoupling of scales hypothesis).

Therefore, it is necessary to introduce an artificial short distance structure in the continuum field integral by modifying the Gaussian measure to restrict the field integration to sufficiently regular fields, continuous to define expectation values of $\sigma^n(x)$, satisfying differentiability conditions to define expectation values involving also derivatives taken at the same point.

This procedure is called in QFT regularization. In the Fourier representation, this modification has the effect of decreasing the contribution of field components corresponding to large momenta.

The impossibility of constructing a model describing the long distance properties without reference to the short distance structure, is a first evidence of non scale-decoupling.

Regularization can be achieved by adding to $\mathcal{H}_{\mathrm{G}}(\sigma)$ terms with higher enough derivatives (a modification that preserves locality but leads, in particle physics, to non-physical short distance singularities):

$$\mathcal{H}_{\mathrm{G}}(\sigma) = \frac{1}{2}\int \mathrm{d}^d x \left[\nabla_x \sigma(x)\right)^2 + r\sigma^2(x)\Big] \\ + \frac{1}{2}\sum_{\ell=2}^{\ell_{\max}} \alpha_\ell \int \mathrm{d}^d x\, \sigma(x)\left(-\nabla_x^2\right)^\ell \sigma(x).$$

For example, simple continuity requires $2\ell_{\max} > d$.

Existence of derivatives of order q requires $2\ell_{\max} > d + q$.

The regularized two-point function is given by

$$\Delta(x) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \, \mathrm{e}^{-ipx} \, \tilde{\Delta}(p)$$

with (taking into account the leading term in the expansion of $B(\sigma)$)

$$\tilde{\Delta}^{-1}(p) = r + b_2 + K(p^2) \text{ with } K(p^2) = p^2 + p^4 \sum_{\ell=2}^{\ell_{\max}} \alpha_\ell p^{2\ell-4}.$$

After regularization

$$\left(\prod_{i=1}^{q} \frac{\partial}{\partial x_{\mu_i}} \right) \Delta(x) \bigg|_{x=0}$$

is defined for all $q < 2\ell_{\max} - d$.

Renormalization group arguments are then required to prove regularization independence (a part of universality) in non-Gaussian theories.

Calculation of the leading correction: the role of dimension 4

In the disordered phase $r > r_c$, in zero field, the magnetization $M = \langle\sigma\rangle$ vanishes and the leading saddle point is simply $\sigma = 0$. The first correction to the steepest descent method then is also the first correction to the Gaussian model.

The corrections to the Gaussian result are obtained by expanding expression (23), separating in the Hamiltonian $\mathcal{H}(\sigma)$ a quadratic part $\mathcal{H}_0(\sigma)$ from a remainder called perturbation:

$$\mathcal{H}(\sigma) = \mathcal{H}_{\mathrm{G}}(\sigma) + \int \mathrm{d}^d x \, B\bigl(\sigma(x)\bigr) = \mathcal{H}_0(\sigma) + \int \mathrm{d}^d x \bigl(B(\sigma(x)) - \tfrac{1}{2} b_2 \sigma^2(x)\bigr)$$

with

$$\mathcal{H}_0(\sigma) = \mathcal{H}_{\mathrm{G}}(\sigma) + \tfrac{1}{2} b_2 \int \mathrm{d}^d x \, \sigma^2(x) \,.$$

The second derivative of the thermodynamic potential is also the inverse of the Fourier transform of the connected two-point function, at vanishing argument.

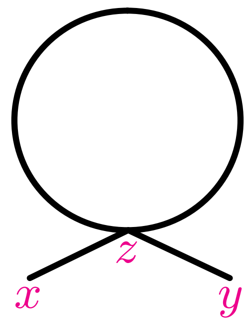

Fig. 4 Feynman diagram: one-loop contribution to the two-point function.

The leading correction to the Gaussian form of the two-point function is then given by the contribution of order b_4 (Fig. 4) generated by the quartic term in $B(\sigma)$:

$$B(\sigma) - \tfrac{1}{2} b_2 \sigma^2 = \frac{1}{4!} b_4 \sigma^4 + O(\sigma^6).$$

Moreover, in zero magnetization the connected two-point function is equal to the complete two-point function. After division by the partition function, one obtains

$$W^{(2)}(x-y) = \langle \sigma(x)\sigma(y) \rangle = \Delta(x-y) - \frac{b_4}{2} \int \mathrm{d}^d z \, \Delta(x-z)\Delta(0)\Delta(z-y) + O(b_4^2).$$

In the Fourier representation, the expression becomes

$$\tilde{W}^{(2)}(k) = \tilde{\Delta}(k) - \tfrac{1}{2} b_4 \Delta(0) \tilde{\Delta}^2(k) + O(b_4^2).$$

In the Fourier representation, the two-point vertex function is simply the inverse of the connected two-point function. Thus,

$$\tilde{\Gamma}^{(2)}(k) = \tilde{\Delta}^{-1}(k) + \tfrac{1}{2} b_4 \Delta(0) + O(b_4^2).$$

Then,

$$\tilde{\Delta}^{-1}(p) = r + b_2 + K(p^2), \quad \Delta(x=0) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \tilde{\Delta}(p).$$

Therefore,

$$\tilde{\Gamma}^{(2)}(k) = K(k^2) + r + b_2 + \tfrac{1}{2} b_4 \int \frac{\mathrm{d}^d p}{(2\pi)^d} \tilde{\Delta}(p) + O(b_4^2)\,. \tag{42}$$

We recall that the coefficient of M^2 in the expansion of the thermodynamic potential density $\mathcal{G}(M)$, which is also the inverse of the magnetic susceptibility in zero field, is given by

$$\chi^{-1}(M=0) = \left.\frac{\partial^2 \mathcal{G}}{(\partial M)^2}\right|_{M=0} = \int \mathrm{d}^d x\, \Gamma^{(2)}(x-y) = \tilde{\Gamma}^{(2)}(k=0).$$

The critical behaviour

We infer the expansion

$$\mathcal{G}''(0) = r + b_2 + \tfrac{1}{2} b_4 \int \frac{\mathrm{d}^d p}{(2\pi)^d} \tilde{\Delta}(p) + O(b_4^2). \tag{43}$$

The criticality condition is now

$$\mathcal{G}''(0) = r_c + b_2 + \tfrac{1}{2} b_4 \int \frac{\mathrm{d}^d p}{(2\pi)^d} \tilde{\Delta}(p) + O(b_4^2) = 0\,. \tag{44}$$

The first effect of the correction is to modify the critical value r_c and, thus, the (non universal) critical temperature. In the term of order b_4, one can replace r_c by $-b_2$, its leading order value, and the equation for r_c becomes

$$0 = r_c + b_2 + \frac{b_4}{2(2\pi)^d} \int \frac{\mathrm{d}^d p}{K(p^2)} + O(b_4^2),$$

Since $K(p^2) \sim p^2$ for $p \to 0$, one verifies again the pathological character of the model in dimension $d = 2$ where the integral diverges at $p = 0$: continuous phase transitions in dimension 2 cannot be described by the Gaussian model and, thus, a perturbed Gaussian model.

We then differentiate $\mathcal{G}''(0)$ with respect to r. At this order we can substitute $b_2 = -r_c$. Thus,

$$\frac{\partial \mathcal{G}''(0)}{\partial r} = 1 - \frac{b_4}{2(2\pi)^d} \int \frac{\mathrm{d}^d p}{[K(p^2) + r - r_c)]^2} + O(b_4^2)\,. \tag{45}$$

If the integral has a finite limit when $r \to r_c$, the derivative exists at $r = r_c$ and the correction to $\mathcal{G}''(0)$, beyond the Gaussian contribution, remains proportional to $r - r_c \propto T - T_c$:

$$\mathcal{G}''(0) \underset{r \to r_c}{\sim} (r - r_c) \left. \frac{\partial \mathcal{G}''(0)}{\partial r} \right|_{r = r_c} .$$

Then, $\mathcal{G}''(0)$ vanishes linearly at the critical point like $T - T_c$, as in the quasi-Gaussian theory, and only the non-universal coefficient is weakly modified.

One finds

$$\left. \frac{\partial \mathcal{G}''(0)}{\partial r} \right|_{r = r_c} = 1 - \frac{b_4}{2(2\pi)^d} \int \frac{\mathrm{d}^d p}{K^2(p^2)} + O(b_4^2) \,, \qquad (46)$$

where, independently of the regularization,

$$K^2(p^2) \underset{p \to 0}{\sim} p^4 .$$

The role of dimension 4. Since $K^2(p^2)$ for $p \to 0$ behaves like p^4, the integral converges only for $d > 4$. We conclude:

For $d > 4$, the perturbation to the Gaussian theory is small, and modifies only non-universal quantities. The magnetic susceptibility still diverges like $1/(T - T_c)$ and the critical exponent γ keeps its Gaussian value: $\gamma = 1$.

For $2 < d \leq 4$, on the contrary, the integral diverges when $r \to r_c$. Thus, however small the amplitude b_4 of the first correction to the Gaussian distribution is, for $d \leq 4$ when the correlation length ξ diverges the contribution of order b_4 eventually becomes larger than the Gaussian term.

For $d \leq 4$, the perturbative expansion is not valid close to T_c, and the universal predictions of the Gaussian model and the perturbed Gaussian model are inconsistent.

It is instructive to evaluate more precisely the behaviour of the integral when $|r - r_c| \ll 1$ for $d < 4$:

$$\frac{\partial \mathcal{G}''(0)}{\partial r} \sim 1 - \frac{b_4}{2(2\pi)^d} \int \frac{\mathrm{d}^d p}{[r - r_c + K(p^2)]^2} + O(b_4^2)\,.$$

For $d < 4$, the integral converges at infinity. Replacing $K(p^2)$ by p^2 modifies the result only by a negligible constant for $r \to r_c$. After the change of variables $p = p' \sqrt{r - r_c}$, the integral becomes

$$\begin{aligned} \frac{1}{(2\pi)^d} \int \frac{\mathrm{d}^d p}{(r - r_c + p^2)^2} &= (r - r_c)^{d/2-2} \frac{1}{(2\pi)^d} \int \frac{\mathrm{d}^d p}{(1 + p^2)^2} \\ &= \frac{\Gamma(2 - d/2)}{(4\pi)^{d/2}} (r - r_c)^{d/2-2}. \end{aligned}$$

Integrating over r and introducing the Gaussian correlation length $\xi = 1/\sqrt{r - r_c}$, one infers

$$\mathcal{G}''(0) = \chi^{-1} \underset{\xi \gg 1}{=} (r - r_c) \left[1 + \frac{b_4}{2} \frac{\Gamma(1 - d/2)}{(4\pi)^{d/2}} \xi^{4-d} \right] + O(b_4^2). \tag{47}$$

(Here, the correlation length is measured in units of the microscopic scale.) For $d = 4$, the correction has a logarithmic divergence that requires a regularization, but the leading logarithmic term does not depend on the regularization parameter:

$$\mathcal{G}''(0) = \chi^{-1} \underset{\xi \gg 1}{=} (r - r_c) \left(1 - \frac{b_4}{16\pi^2} \ln \xi \right) + O(b_4^2).$$

These expressions relate explicitly the failure of the quasi-Gaussian approximation to the divergence of the correlation length.

To summarize:

i) For dimensions $d > 4$, the correction does not modify the universal predictions of the quasi-Gaussian approximation. One finds some singular corrections but they yield sub-leading contributions.

(ii) For dimensions $d \le 4$, singularities, also called 'infra-red'(IR) a denomination borrowed from QFT, consequences of the large distance behaviour of the Gaussian two-point function, or at vanishing argument of its Fourier transform, imply that the Gaussian predictions cannot be correct in general.

An inspection of higher order corrections confirms these results. For $d > 4$ the corrections are less and less singular, which confirms the validity of the first order analysis whereas for $d \le 4$, they are increasingly singular when the order increases. Moreover, at each order, close to four dimensions $\int \mathrm{d}^d x\, \sigma^4(x)$ gives the leading contribution.

The perturbative terms responsible for this difficulty involve the ratio ξ between the correlation length and the microscopic scale.

This gives some indication about the mechanism responsible for the failure of the quasi-Gaussian approximation: physics at the microscopic scale does not decouple from physics at large distance.

Indeed, for $d > 4$, the contribution from arguments $|p| \le \xi^{-1}$ is negligible when ξ diverges, which means that in direct space the degrees of freedom corresponding to distances of the order of the correlation length or larger play a negligible role.

On the contrary, for $d \le 4$, at T_c, all scales contribute. This property invalidates ideas based on the central limit theorem, namely that a small number of degrees of freedom with a quasi-Gaussian distribution can replace the infinite number of initial microscopic degrees of freedom.

To solve this problem of coupling between all scales, a new tool has been invented, the renormalization group.

Note that the first singular contribution depends only on the coefficient of σ^4 in the expansion of $B(\sigma)$ and on the asymptotic form of the propagator (the Gaussian two-point function) at large distance or small momenta. The short distance modification has only ensured large momentum convergence.

A systematic study then confirms that the most singular terms in each order of the perturbative expansion can be reproduced, in the critical limit, by a statistical field theory with an interaction of σ^4 type, in continuum Euclidean space.

Therefore, if the sum of the most divergent terms to all orders is the leading contribution, then the existence of a continuum limit and some universal properties follow, since then the corresponding field theory depends only on a small number of parameters.

Finally, the consistency of the analysis can again be verified by evaluating the leading corrections.

From Gaussian models to Renormalization Group

We have studied Ising type models (but the study can be easily extended to ferromagnetic models with $O(N)$ symmetry) with short range interactions and determined the behaviour of the thermodynamic functions near a continuous phase transition, within the framework of the quasi-Gaussian or mean field approximations.

We have shown that these approximations predict a set of universal properties, that is, properties independent of the detailed structure of interactions or microscopic Hamiltonians, including dimension of space or symmetries.

However, many experimental observations as well as numerical and analytical results coming from model systems show that such results cannot be quantitatively correct, at least in dimensions 2 or 3.

For example, the exact solution of the Ising model in two dimensions yields exponents like $\beta = 1/8$, $\eta = 1/4$ or $\nu = 1$, clearly different from the predictions of the quasi-Gaussian approximation.

By examining the leading corrections to the Gaussian approximation, we have identified the origin of the difficulty.

Above dimension 4 these corrections do not affect universal quantities; by contrast, below four dimensions, the corrections diverge at the critical temperature and, thus, invalidate the assumptions that are at the basis of the quasi-Gaussian approximation.

The analysis also indicates that the coupling of degrees of freedom corresponding to very different length scales plays an essential role: it is impossible to consider only effective macroscopic degrees of freedom.

One could then fear that physics in dimension $d \leq 4$, even at large distance, is sensitive to the detailed microscopic structure of systems.

However, surprisingly, some universal properties survive, though different from those of the quasi-Gaussian approximation.

Moreover, these properties are less universal: statistical systems that have the same properties in the quasi-Gaussian approximation, divide into universality classes characterized by the dimension of space, symmetries and some other qualitative features.

To explain this somewhat paradoxical situation, a completely new tool, initially suggested by Kadanoff (1966), has been developed by Wilson (1971), Wegner..., and then many other physicists, the Renormalization Group (RG) (different in spirit and more general than the earlier RG of quantum field theory).

In this approach, the RG is generated by integrating successively over the degrees of freedom corresponding to the shortest scales.

One then obtains a sequence of models which all describe the same large distance physics but in which details of the short distance structure are gradually eliminated.

If this sequence has a limit, which implies that the RG transformations admit fixed points, then universality properties are explained: all statistical models which, after these repeated transformations, converge toward the same fixed point, belong to the same universality class.

Stated in this general form, the general ideas of RG are extremely suggestive but somewhat vague. The main issue becomes the implementation and this is a non trivial issue.

First, one has to define precisely the way one integrates over short-distance degrees of freedom. Then this general RG remains difficult to set-up because it acts on the infinite dimensional space of possible statistical models. In the simplest implementation, in the continuum, it leads to quadratic functional equations.

Only Gaussian models can be discussed systematically. One can identify the simplest fixed point, the Gaussian fixed point, which belongs to the class of Gaussian models discussed previously.

Moreover, a complete local stability analysis of the Gaussian fixed point is possible. It allows classifying all perturbations as relevant, that is, which become increasingly important at large distance, irrelevant in the opposite case and marginal in the limiting situation.

More generally, in this framework, the RG of quantum field theory appears as an asymptotic form of the general renormalization when one applies it to the neighbourhood of a Gaussian fixed point.

In the specific context of QFT, the assumptions at the basis of the RG have been clarified. The analysis has confirmed the major relation, initially recognized by Wilson, between the quantum field theory describing the fundamental physics at the microscopic scale and the theory of the macroscopic critical phenomena.

QFT techniques combined with RG could then be used to discuss phase transitions and to calculate universal quantities, like critical exponents.

The renormalization group: General idea

To construct a RG flow in continuum space, the basic idea is to integrate in the field integral recursively over short distance degrees of freedom.

This procedure generates a sequence of effective Hamiltonians $\mathcal{H}_\lambda$ function of a scale parameter $\lambda > 0$ (such that $\mathcal{H}_1 = \mathcal{H}$), related by a transformation $\mathcal{T}$ acting in the space of Hamiltonians such that

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \mathcal{H}_\lambda = \mathcal{T}\left[\mathcal{H}_\lambda\right], \tag{48}$$

a flow equation called RG equation (RGE).

The appearance of the derivative $\lambda \mathrm{d}/\mathrm{d}\lambda = \mathrm{d}/\mathrm{d}\ln\lambda$ reflects the multiplicative character of dilatations. The RGE thus defines a dynamical process in the 'time' $\ln\lambda$. The denomination renormalization group (RG) refers to the property that $\ln\lambda$ can be considered as an element of the additive group of real numbers.

RG equation: General structure, fixed points

One looks for a RG flow that defines a stationary Markov process, that is, $\mathcal{T}[\mathcal{H}_\lambda]$ depends on $\mathcal{H}_\lambda$ but not on the trajectory that has led from $\mathcal{H}_{\lambda=1}$ to $\mathcal{H}_\lambda$, and depends on λ only through $\mathcal{H}_\lambda$.

Universality is then related to the existence of fixed points, solution of

$$\mathcal{T}(\mathcal{H}^*) = 0\,.$$

One also assumes that the mapping $\mathcal{T}$ is differentiable so that, near a fixed point, the RG flow can be linearized,

$$\mathcal{T}(\mathcal{H}^* + \Delta\mathcal{H}_\lambda) \sim L^* \Delta\mathcal{H}_\lambda\,,$$

and is governed by the eigenvalues and eigenvectors of the linear operator L^*. Formally, the local solution of the linearized equations can be written as

$$\mathcal{H}_\lambda = \mathcal{H}^* + \lambda^{L^*}\left(\mathcal{H}_{\lambda=1} - \mathcal{H}^*\right).$$

Eigenvalues and local stability

Global stability cannot be investigated in general, but local stability near the fixed point can be studied by determining the spectrum of L^*.

We consider here only the situation where the spectrum of L^* is real, a property true for the simple systems we consider but not proved in general.

In the example of the random walk, we have already introduced the RG terminology:

(i) Positive eigenvalues correspond to directions of instability and the corresponding eigenoperators are called relevant.

(ii) Vanishing eigenvalues correspond to marginal operators. Then, the linearized flow is in general no longer sufficient to determine whether the perturbation corresponds to a marginally stable or unstable situation.

An expansion of the RG flow to second order in the perturbation to the fixed point is required and this leads in general to a logarithmic behaviour.

A special case of vanishing eigenvalues corresponds to redundant operators, which merely correspond to a simple change of parametrization.

(iii) Negative eigenvalues correspond to irrelevant operators and to directions of stability.

The concept of universality is meaningful when only a small number of operators are relevant.