PHASE TRANSITIONS WITH NONSTANDARD CRITICAL BEHAVIOR*

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We discuss phase transitions and critical behavior deviating from the standard scheme based on a mean-field theory renormalizing only the mass of the critical excitations completed with a perturbative scaling renormalization of the interaction strength. On examples of mean-field theories for spin glasses and for quantum phase transitions we show that coupling constants are relevant variables in these systems and are to be renormalized already within the mean-field approximations.

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1. Introduction

Statistical many-particle systems can exhibit different equilibrium states characterized by a number of macroscopic "order" parameters. Varying external conditions, such as temperature, pressure, magnetic field *etc.*, we can force the system to change the symmetry of the equilibrium state and to pass from one state to another. If the symmetry and the order parameters change continuously we speak about continuous phase transitions. They are characterized by nonanalyticities in thermodynamic potentials or singularities in correlation functions, *i.e.*, derivatives of the free energy. Critical points, where two or more phases meet, are hence accessible only by nonperturbative methods. To describe the asymptotic behavior near the critical points is one of the boldest challenges of statistical mechanics, since even the simplest microscopic models are not exactly solvable apart from a few exceptions.

Modern theory of critical phenomena is based on extraordinary features of continuous transitions such as scaling, universality and the renormalization group [1]. The theory of renormalizations that has developed from these

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concepts is at present the most advanced and sophisticated tool we have at hand to study and understand critical behavior. To be able to employ the scaling ideas and the renormalization group the system must obey specific assumptions that can be called standard criticality. However, not all phase transitions we observe and study fit the standard scheme. It is the aim of this lecture to demonstrate on a few examples what problems we are facing in cases that cannot be transformed to standard models of critical behavior. We use two examples of phase transitions, one from classical and one from quantum statistical mechanics, on which we demonstrate that even a mean-field approximation does not obey the Landau criteria without which we cannot apply the standard renormalization scheme.

2. Standard critical behavior

Critical points cannot be treated perturbatively and we always have to start with a nonperturbative solution of a microscopic model. The simplest solution providing a first quantitative information about phase transitions and critical phenomena is a mean-field approximation. It is usually introduced as a saddle-point approximation to a free-energy functional reducing it to the Landau–Ginzburg expansion in the order parameter φ of the Gibbs free energy that in momentum space reads

$$\begin{aligned}\Phi[\varphi] \;&=\; \frac{1}{2}\sum_{\boldsymbol{q}}(\mu(T)^2+\alpha^2q^2)|\varphi(\boldsymbol{q})|^2 \\ &\quad+\frac{\lambda}{4!N^2}\sum_{\boldsymbol{q}_i}\varphi(\boldsymbol{q}_1)\varphi(\boldsymbol{q}_2)\varphi(\boldsymbol{q}_3)^*\varphi(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q}_3)^* . \end{aligned} \tag{1}$$

Equilibrium solution is then obtained as a minimum of functional (1) with respect to the variable $\varphi(\boldsymbol{q})$. The critical point is defined from vanishing of the bare mass of the excitations $\mu^2 \to 0$. A two-point correlation function, being the inverse of the quadratic part of the r.h.s. of Eq. (1), diverges in the long-wavelength limit $[\mu(T)^2+\alpha^2q^2]^{-1} \underset{q\to 0}{\longrightarrow} \infty$. The first important conclusion is that the mean-field approximation defines a diverging correlation length $\xi(T)=\mu(T)^{-1}\to\infty$ from the diverging two-point propagator.

In the ordered phase the bare mass $\mu^2<0$ and we have to renormalize it so that the effective mass remains positive even in the ordered state: $\mu^2 \to m^2 = \mu^2 + \frac{\lambda}{6}|\varphi|^2$. The mean-field theory must renormalize the mass of the critical excitations. There is, however, no need for renormalization of the interaction constant within the mean-field solution. The coupling constant hence remains irrelevant in the mean-field picture.

Mean field is a nonperturbative approximation enabling to deal with the singularities at the critical point. If it encompasses all divergences, it becomes asymptotically exact in the critical region. It is the case in high spatial dimensions, above the upper critical dimension d_u, with many nearest neighbors. However, in dimensions $d < d_u = 4$ fluctuations around the mean-field order parameter get singular and new divergences emerge. Interaction constant λ (charge) becomes relevant and must be renormalized $\lambda \to g = \Gamma(0,0,0)$ along with the mass to treat critical behavior properly. Here Γ is a four-point vertex function. This is achieved via a renormalized perturbation expansion using scaling arguments and eventually with the aid of the renormalization group [2]. Introducing the renormalized dimensionless running coupling constant $\widehat{g} = gm^{d-4}$ we succeed to factorize all the divergences as powers of the only diverging correlation length ξ introduced in the mean-field theory. The factorization enables one to single out the divergent contributions, which leads to a universal behavior. Moreover, the fixed point of the renormalized perturbation theory for the universal quantities (critical exponents) remains in the weak-coupling regime, *i.e.*, $\widehat{g}_c \ll 1$.

3. Nonstandard critical behavior with classical statistics

The standard description of critical behavior outlined in the preceding section can break down in more complex situations from various reasons. First problem we may encounter is the specification of the relevant macroscopic phase space (order parameters) for the possible equilibrium states. If our phase space is not large enough we end up with an unstable solution. We demonstrate that this is the case when the standard approach is applied to spin–glass models.

3.1. Mean-field theory of spin glasses — naive approach

The simplest model of spin glasses is a random-bond Ising model (Edwards–Anderson model). The averaged free energy is obtained from the averaging over the thermal fluctuations and then over the configurations of the spin–spin coupling that is assumed a Gaussian random variable. A global mean-field theory can be constructed from the limit $d \to \infty$. The free energy for one configuration of the spin–spin coupling reduces in $d = \infty$ to the Thouless–Anderson–Palmer (TAP) representation with local magnetizations m_i and internal magnetic fields η_i as order (variational) parameters

$$\begin{aligned} -\beta F \ = \ & \frac{1}{2}\sum_{i,j}\beta J_{ij}m_i m_j + \frac{1}{4}\sum_{i,j}\beta^2 J_{ij}^2(1-m_i^2)(1-m_j^2) \\ & - \sum_i \beta m_i \eta_i + \sum_i \ln 2\cosh\beta\,(h+\eta_i) \qquad (2) \end{aligned}$$

with $\beta = 1/k_{\rm B}T$. At equilibrium the internal magnetic field is defined as a sum of an external field h and a local magnetizations and in the leading $d \to \infty$ asymptotics it becomes a Gaussian random variable

$$\begin{aligned} \eta_i &= \sum_j J_{ij}\left[m_j - m_i\beta J_{ij}(1-m_j^2)\right] , \\ \langle \eta_i\eta_j\rangle_{\rm av} &= \delta_{i,j}\sum_l J_{il}^2 m_l^2 = \delta_{i,j}J^2 q_{\rm EA} , \end{aligned} \tag{3}$$

where $q_{\rm EA}$ is the Edwards–Anderson order parameter and the averaging is over the local random variables η_i. Performing the averaging of the TAP over configurations of the spin–spin coupling J_{ij} we end up with the Sherrington–Kirkpatrick (SK) solution with the only macroscopic, translationally invariant parameter $q_{\rm EA} = \langle m_i^2\rangle_{\rm av}$. This solution is, however, unstable at low temperatures, since the macroscopic phase space to which we reduced the problem in the mean-field approximation is too small [3].

3.2. Mean-field theory of spin glasses — sophisticated approach

To extend the macroscopic phase space in the Sherrington–Kirkpatrick model we can either try to average the TAP free energy numerically and work with nonlocal quantities or we have to improve our reduction of the problem to a single-site theory in a more sophisticated way. Parisi proposed the well-known replica-symmetry breaking solution within the replica approach to the averaging procedure where he introduced an order-parameter function $q(x)$, $x \in [0,1]$ with the property $q_{\rm EA} = q(1)$ [4]. This solution contains a rather artificial mathematical trick the physical meaning of which has not been fully understood.

A more direct way to find the relevant macroscopic phase space in translationally invariant (averaged) local variables is to utilize the notion of the so-called real replicas [5]. The idea of real replicas is based on the existence of a number of quasi-equilibrium solutions in the spin–glass phase. We ascribe to each solution independent spin variables and hence replicate the initial spin Hamiltonian. We further introduce an infinitesimal coupling μ^{ab} between the replicas $\Delta H = \frac{1}{2}\sum_{a\neq b}\sum_i \mu^{ab}S_i^a S_i^b$. After averaging over thermal fluctuations we obtain a TAP-like free energy with ν real replicas

$$\begin{aligned} -\beta F_\nu = \sum_{a=1}^{\nu}\Bigg\{ & \frac{1}{2}\sum_{i,j}\beta J_{ij}m_i^a m_j^a + \frac{1}{4}\sum_{i,j}\beta^2 J_{ij}^2\left[1-(m_i^a)^2\right]\left[1-(m_j^a)^2\right] \\ & - \sum_i m_i^a\left[\beta\eta_i^a + (\beta J)^2\sum_{b=1}^{a-1}\chi^{ab}m_i^b\right] - \frac{1}{2}N(\beta J)^2\sum_{b=1}^{a-1}(\chi^{ab})^2\Bigg\} \end{aligned}$$

$$+\sum_i \ln \mathrm{Tr} \exp\left\{\frac{1}{2}(\beta J)^2 \sum_{a\neq b}^{\nu} \chi^{ab} S_i^a S_i^b + \beta \sum_{a=1}^{\nu} \left(h+\eta_i^a\right) S_i^a\right\} . \qquad (4)$$

This free energy contains except for the local magnetizations m_i^a and internal magnetic fields η_i^a also averaged overlap local susceptibilities $\chi^{ab} = \langle\langle S_i^a S_i^b\rangle\rangle_{\mathrm{av}} - \langle m_i^a\rangle_{\mathrm{av}}\langle m_i^b\rangle_{\mathrm{av}}$, $(a \neq b)$ as order parameters. The internal magnetic fields are again Gaussian random variables

$$\begin{aligned}\eta_i^a &= \sum_j J_{ij} m_j^a - \beta J^2 \sum_{b=1}^{\nu} m_i^b \chi^{ab} ,\\ \langle \eta_i^a \eta_j^b\rangle_{\mathrm{av}} &= \delta_{i,j} \sum_l J_{il}^2 m_l^a m_l^b = \delta_{i,j} J^2 q^{ab} ,\end{aligned} \qquad (5)$$

where $q^{aa} = q_{\mathrm{EA}}$. Free energy (4) can in principle be directly averaged with definitions (5). However, the number of real replicas ν is not fixed and in fact it must be infinite for the equilibrium state [5]. The limit $\nu \to \infty$ can be reached without Ansatz only successively through finite number of replicas. Only in this way we can guess the symmetry in the phase space with q^{ab} and χ^{ab} as order parameters. It is straightforward to derive explicit formulas for the case of two real replicas. The averaged free energy density reads

$$\begin{aligned}2f_2 &= -\frac{\beta}{2}(1-q_0)^2 + \beta\chi_1\left(q_1 + \frac{\chi_1}{2}\right)\\ &\quad -\frac{1}{\beta}\int \frac{d\xi_1 d\xi_2}{2\pi} \exp\left\{-\frac{\xi_1^2+\xi_2^2}{2}\right\} \ln 2\left\{e_+ c_+ + e_- c_-\right\} ,\end{aligned} \qquad (6)$$

where we set $J = 1$ and denoted $e_\pm = \exp\{\pm\beta^2\chi_1\}$ and

$$\begin{aligned}c_+ &= \cosh\left[\beta\left(2h + \sqrt{q_0 - \frac{q_1^2}{q_0}}\,\xi_1 + \left(\sqrt{q_0} + \frac{q_1}{\sqrt{q_0}}\right)\xi_2\right)\right] ,\\ c_- &= \cosh\left[\beta\left(\sqrt{q_0 - \frac{q_1^2}{q_0}}\,\xi_1 - \left(\sqrt{q_0} - \frac{q_1}{\sqrt{q_0}}\right)\xi_2\right)\right] .\end{aligned}$$

Stationarity equations for the variational parameters q_0, q_1 and χ_1 are easily derived. The actual order parameters in the low-temperature phase are χ_1 and $\Delta_1 = q_0 - q_1$ determining the de Almeida–Thouless (AT) instability line.

One can easily verify that below the AT line the SK solution ($\Delta_1 = \chi_1 = 0$) is unstable and different real replicas are coupled. However, even the simplest mean-field approximation beyond SK does not fit the standard scheme of critical behavior. First, there is no apparent divergent propagator from which we could read off the diverging correlation length. Second, the mean-field approximation renormalizes simultaneously both effective mass (averaged squared magnetization) and the interaction strength (overlap susceptibility). Third, the free energy is not symmetric w.r.t. reflection $f_2(\chi_1) \neq f_2(-\chi_1)$ and the Landau expansion does not hold. Last, but not least, the free energy is maximized w.r.t. q_0, Δ_1 and minimized w.r.t. χ_1. We are facing a delicate mini–max problem where we have to find a state with the lowest free energy among the stable states.

4. Mean-field description of quantum phase transitions

Quantum phase transitions, in particular in itinerant models of interacting fermions, display critical behavior with anomalous properties, since the transitions are not driven by temperature but by the interaction strength. Hence from the very beginning the coupling constant becomes a relevant variable that must be renormalized even in the mean-field approximation. We thus have a significant deflection from the standard scheme. We show on the example of a transition to the spin-flip state (transverse antiferromagnetic order in an external magnetic field) that one has to renormalize two-particle vertex functions (effective interaction) so as to construct a mean-field theory of the Landau type beyond the weak-coupling regime.

4.1. Weak-coupling limit

The only existing mean-field theory for quantum phase transitions with two or more relevant non-commuting operators is the BCS theory of the superconducting phase [6]. It is the standard weak-coupling mean-field theory as in classical physics with the exception that it does not define a diverging two-point correlation function.

To describe a transverse magnetic order of the Hubbard model in an external magnetic field with two relevant non-commuting operators $S^z, S^\pm$ we use the Nambu spinor formalism to account for anomalous propagators that do not conserve spin. We introduce Nambu spinors

$$\Psi_{\boldsymbol{Q},\boldsymbol{k}} = \left(c_{\boldsymbol{Q}/2+\boldsymbol{k}\uparrow} \right) c_{\boldsymbol{Q}/2-\boldsymbol{k}\downarrow}, \quad \Psi^\dagger_{\boldsymbol{Q},\boldsymbol{k}} = \left(c^\dagger_{\boldsymbol{Q}/2+\boldsymbol{k}\uparrow} \; c^\dagger_{\boldsymbol{Q}/2-\boldsymbol{k}\downarrow} \right) \tag{7}$$

and a propagator being a 2×2 matrix

$$G_{\boldsymbol{Q}}(\boldsymbol{k}, z) = \frac{1}{(z + x^\uparrow_{\boldsymbol{k}})(z + x^\downarrow_{-\boldsymbol{k}}) - \eta^\perp_{\boldsymbol{Q}} \bar{\eta}^\perp_{\boldsymbol{Q}}} \begin{bmatrix} z + x^\downarrow_{-\boldsymbol{k}} & \eta^\perp_{\boldsymbol{Q}} \\ \bar{\eta}^\perp_{\boldsymbol{Q}} & z + x^\uparrow_{\boldsymbol{k}} \end{bmatrix} . \tag{8}$$

We used an abbreviation $x^\sigma_{\boldsymbol{k}} := (\mu - \frac{U}{2} n) + \sigma(B + \frac{U}{2} m) - \varepsilon(\boldsymbol{Q}/2 + \sigma\boldsymbol{k})$. Here μ is the chemical potential, U is the Hubbard screened interaction, and $\varepsilon(\boldsymbol{k})$ stands for the lattice dispersion relation. Momentum $\boldsymbol{Q}$ determines propagation of the "Cooper pair", n, m are the particle occupation and magnetization in the Hartree approximation, and $\eta^{\perp}_{\boldsymbol{Q}}$ is the anomalous order parameter describing the ordered phase.

The mean-field theory in the weak-coupling regime amounts to the Hartree decoupling that in the Nambu formalism leads to a BCS equation

$$\eta^{\perp}_{\boldsymbol{Q}} = \eta^{\perp}_{\boldsymbol{Q}} \frac{U}{N} \sum_{\boldsymbol{k}} \left(\frac{f(E^{+}_{\boldsymbol{Q},\boldsymbol{k}})}{E^{+}_{\boldsymbol{Q},\boldsymbol{k}}} - \frac{f(E^{-}_{\boldsymbol{Q},\boldsymbol{k}})}{E^{-}_{\boldsymbol{Q},\boldsymbol{k}}} \right) \tag{9}$$

with a new dispersion $2E^{\pm}_{\boldsymbol{Q},\boldsymbol{k}} = -(x^{\uparrow}_{\boldsymbol{k}} + x^{\downarrow}_{-\boldsymbol{k}}) \pm \sqrt{(x^{\uparrow}_{\boldsymbol{k}} - x^{\downarrow}_{-\boldsymbol{k}})^2 + 4\eta^{\perp}_{\boldsymbol{Q}}\bar{\eta}^{\perp}_{\boldsymbol{Q}}}$, N denotes the number of lattice sites.

4.2. Quantum phase transitions beyond weak coupling

BCS mean-field approximation from the preceding subsection fits the Landau mean-field approach to continuous transitions only in the weak-coupling regime $U \to 0$, since it uses the Hartree decoupling. In this limit the quantum fluctuations are suppressed, since interaction cannot be used as a parameter controlling the transition. Genuine quantum criticality lies beyond the weak-coupling regime. To construct an adequate mean-field theory we have to go beyond the Hartree decoupling. In fact we have to renormalize two-particle vertex functions. In intermediate coupling one can use the so-called FLEX approximations summing multiple two-particle scatterings of the same type [7]. To this purpose we need two-particle propagators. The electron–hole propagator in the Nambu formalism becomes a 4×4 matrix that can be represented as

$$Y^{\sigma\sigma'}_{\eta\eta'}(\boldsymbol{q}, i\nu_m) = \frac{1}{\beta N} \sum_{\boldsymbol{k}n} G^{\sigma\sigma'}(\boldsymbol{k}+\boldsymbol{q}, i\omega_n + i\nu_m) G_{\eta\eta'}(\boldsymbol{k}, i\omega_n)\ . \tag{10}$$

Here $\omega_n = (2n+1)\pi$, $\nu_m = 2m\pi$ are fermionic and bosonic Matsubara frequencies, respectively. The one-particle propagators are no longer the Hartree ones and we have

$$G(\boldsymbol{k}, z) = \frac{1}{D(\boldsymbol{Q}; \boldsymbol{k}, z)} \begin{bmatrix} z + x^{\downarrow}_{\boldsymbol{Q}}(\boldsymbol{k}, z) & \eta^{\perp}_{\boldsymbol{Q}}(\boldsymbol{k}, z) \\ \bar{\eta}^{\perp}_{\boldsymbol{Q}}(\boldsymbol{k}, z) & z + x^{\uparrow}_{\boldsymbol{Q}}(\boldsymbol{k}, z) \end{bmatrix} \tag{11}$$

with $D(\boldsymbol{Q}; \boldsymbol{k}, z) = (z + x^{\uparrow}_{\boldsymbol{Q}}(\boldsymbol{k}, z))(z + x^{\downarrow}_{\boldsymbol{Q}}(\boldsymbol{k}, z)) - \eta^{\perp}_{\boldsymbol{Q}}(\boldsymbol{k}, z)\bar{\eta}^{\perp}_{\boldsymbol{Q}}(\boldsymbol{k}, z)$ and $x^{\sigma}_{\boldsymbol{Q}}(\boldsymbol{k}, z) := \mu + \sigma B - \varepsilon(\boldsymbol{Q}/2 + \sigma\boldsymbol{k}) - \Sigma^{\sigma}_{\boldsymbol{Q}}(\boldsymbol{k}, z)$. For consistence we had to introduce one-electron normal and anomalous self-energies Σ and $\eta^{\perp}$.

The generating functional for the interacting part of the grand potential in the FLEX approximation can be formally represented as

$$f_U = \frac{1}{2\beta N} \sum_{\boldsymbol{q}m} \left\{ \mathrm{Tr}\ln\left[1 + \widehat{UY}(\boldsymbol{q}, i\nu_m)\right] + \frac{1}{4}\mathrm{Tr}\ \widehat{UY}(\boldsymbol{q}, i\nu_m)\widehat{UY}^{\dagger}(\boldsymbol{q}, i\nu_m) \right\}, \tag{12}$$

where the interaction (two-particle vertex) matrix explicitly is

$$\left(\widehat{UY}\right)^{\sigma\sigma'}_{\eta\eta'} := U \begin{bmatrix} -Y^{\downarrow\uparrow}_{\downarrow\uparrow} & -Y^{\downarrow\uparrow}_{\downarrow\downarrow} & -Y^{\downarrow\downarrow}_{\downarrow\uparrow} & -Y^{\downarrow\downarrow}_{\downarrow\downarrow} \\ Y^{\uparrow\uparrow}_{\downarrow\uparrow} & Y^{\uparrow\uparrow}_{\downarrow\downarrow} & Y^{\uparrow\downarrow}_{\downarrow\uparrow} & Y^{\uparrow\downarrow}_{\downarrow\downarrow} \\ Y^{\downarrow\uparrow}_{\uparrow\uparrow} & Y^{\downarrow\uparrow}_{\uparrow\downarrow} & Y^{\downarrow\downarrow}_{\uparrow\uparrow} & Y^{\downarrow\downarrow}_{\uparrow\downarrow} \\ -Y^{\uparrow\uparrow}_{\uparrow\uparrow} & -Y^{\uparrow\uparrow}_{\uparrow\downarrow} & -Y^{\uparrow\downarrow}_{\uparrow\uparrow} & -Y^{\uparrow\downarrow}_{\uparrow\downarrow} \end{bmatrix}. \tag{13}$$

We can now expand (12) in lowest orders of the anomalous functions (order parameters) and obtain a Landau-like dynamical mean-field theory of quantum phase transitions for intermediate coupling. The defining mean-field equation becomes a homogeneous integral equation for the anomalous function $\eta^{\perp}_{\boldsymbol{Q}}(\boldsymbol{k}, i\nu_m)$. BCS equation (9) is revealed only in linear order of the interaction strength U.

5. Conclusions

We tried to demonstrate that although the standard renormalization approach to critical phenomena consisting of mean-field & scaling is a powerful tool it is far from being complete. There are a number of situations where this scheme breaks down. Such a situation occurs when the interaction constant becomes relevant in the critical region from the very beginning. We are then unable to extract a diverging correlation length from the two-point propagator and have to renormalize simultaneously both the mass and the interaction strength in the mean-field approach. This situation does not fit the standard scheme and new techniques must be developed to deal with this criticality. Not even is clear whether in nonstandard transitions we reveal a universal behavior, since divergent contributions to the two-particle functions cannot be decoupled from the finite, regular terms [8].

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