Eur. Phys. J. B **33**, 273–277 (2003)
DOI: 10.1140/epjb/e2003-00166-7

THE EUROPEAN PHYSICAL JOURNAL B

# Gaussian Effective Potential and superconductivity

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Received 18 November 2002 / Received in final form 26 March 2003
Published online 20 June 2003 – 

**Abstract.** The Gaussian Effective Potential in a fixed transverse unitarity gauge is studied for the static three-dimensional U(1) scalar electrodynamics (Ginzburg-Landau phenomenological theory of superconductivity). In the broken-symmetry phase the mass of the electromagnetic field (inverse penetration depth) and the mass of the scalar field (inverse correlation length) are both determined by solution of the coupled variational equations. At variance with previous calculations, the choice of a fixed unitarity gauge prevents from the occurrence of any unphysical degree of freedom. The theory provides a nice interpolation of the experimental data when approaching the critical region, where the standard mean-field method is doomed to failure.

**PACS.** 74.40.+k Fluctuations (noise, chaos, nonequilibrium superconductivity, localization, etc.) – 11.15.Ex Spontaneous breaking of gauge symmetries – 74.20.De Phenomenological theories (two-fluid, Ginzburg-Landau, etc.) – 11.15.Tk Other nonperturbative techniques

## 1 Introduction

Since the discovery of high $T_c$ superconductors several unconventional models have been proposed in order to describe the unusual properties of cuprates. In particular, the strong electron-electron coupling characterizing such materials requires new theoretical methods beyond the standard mean field approach. On the other hand the general phenomenology is still well described by the standard Anderson-Higgs mechanism: the supercurrent is carried by pairs of charged fermions whose non-vanishing expectation value breaks the gauge symmetry, thus endowing the gauge bosons with a mass. Thus the standard Ginzburg-Landau (GL) effective Lagrangian still provides the best framework for a general description of the high-$T_c$ cuprates phenomenology. Moreover, as the GL action can be seen as a power expansion of the exact action around the critical point, the GL action must be recovered by any microscopic theory at least around the transition. Thus, regardless of the nature of the pairing mechanism, the GL action is a sound starting point for a general description of the high-$T_c$ materials. Of course we cannot trust the mean-field approach to the GL effective theory, and we expect that many unconventional properties are connected with the breaking down of the simple mean field picture. Quite recently, the GL model has been extensively studied both theoretically [1,2] and numerically [3] in order to clarify the universality class of the superconducting transition and the role of the critical fluctuations in the high-$T_c$ cuprates, as well as the order of the transition itself [4].

Actually the high-$T_c$ cuprate superconductors are characterized by a very small correlation length $\xi$ which allows the experimentalists to get closer to the critical point where the thermal fluctuations cannot be neglected and the mean field approximation is doomed to fail [5]. As far as we know there is no full evidence that the universal critical behaviour has been reached in any real sample [6], but it is out of doubt that an intermediate range of temperature is now accessible, where thermal fluctuations are not negligible even if the sample is still out of the truly critical regime. Thus, in order to describe some unconventional properties of the high-$T_c$ superconductors, we need to incorporate the role of thermal fluctuations, but unfortunately we cannot rely on the standard renormalization group methods which would only describe the universal limiting behaviour that could not be observed yet in any real sample. We need some kind of interpolation scheme for the non-universal regime where the behaviour depends on the physical parameters of the sample, and we would prefer a non-perturbative method in order to deal with any strong coupling.

In this paper we study the Gaussian fluctuations by means of a variational method, the Gaussian Effective Potential (GEP), which has been discussed by several authors as a tool for describing the breaking of symmetry in a simple scalar theory [7,8]. As a toy model for electro-weak

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interactions, the scalar electrodynamics in four dimensions has been studied by Ibañez-Meier *et al.* [9] who computed the GEP by use of a general covariant gauge. However their method gives rise to an unphysical, and undesirable, degree of freedom.

We compute the GEP for the U(1) scalar electrodynamics in three space dimensions where it represents the standard static GL effective model of superconductivity. In order to make evident the physical content of the theory, thus avoiding the presence of unphysical degrees of freedom, we work in unitarity gauge. This has been shown to be formally equivalent to a full gauge-invariant method once all the gauge degrees of freedom have been integrated out [10]. The variational method provides a way to evaluate both the correlation length $\xi$ and the penetration depth $\ell$ as a solution of coupled equations. The GL parameter $\kappa_{\rm GL} = \ell/\xi$ is found to be strongly temperature dependent in contrast to the simple mean-field description [11]. On the other hand the model predictions are in perfect agreement with some recent experimental data [12], which can be nicely interpolated by our variational calculation.

The comparison with the experimental data is of special importance as it provides a test for the GEP variational method itself. The predictions of the method in 3+1 dimensions, in the context of electro-weak interactions, have been discussed by several authors [7,9,13,14], but no real comparison with experimental data will be achievable until the detection of the Higgs boson. Thus high-$T_c$ cuprate superconductors represent our next best choice in order to test the reliability of the method.

The paper is organized as follows: in Section 2 the GL action and partition function are introduced and discussed within the unitarity gauge; in Section 3 the Gaussian variational method is applied to the three-dimensional GL model, and the coupled variational equations are derived; finally, in Section 4 the phenomenological predictions of the method are compared with some experimental data for the GL parameter.

## 2 The GL action in unitarity gauge

Let us consider the standard static GL action [15]

$$S = \int \mathrm{d}^3x \left[\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}(D_\mu\phi)^*(D^\mu\phi) + \frac{1}{2}m_B^2\phi^*\phi + \lambda_B(\phi^*\phi)^2\right]. \quad (1)$$

Here $\phi$ is a complex (charged) scalar field, whose covariant derivative is defined as

$$D_\mu\phi = \partial_\mu + \mathrm{i}e_B A_\mu \quad (2)$$

and $\mu, \nu = 1, 2, 3$ run over the three space dimensions. The magnetic field components $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ satisfy

$$\frac{1}{2}F_{\mu\nu}F^{\mu\nu} = |\nabla \times \mathbf{A}|^2 \quad (3)$$

and the partition function is defined by the functional integral

$$Z = \int D[\phi, \phi^*, A_\mu]\mathrm{e}^{-S}. \quad (4)$$

We may assume a transverse gauge $\nabla \cdot \mathbf{A} = 0$, and then switch to unitarity gauge in order to make $\phi$ real. Let us define two real fields $\rho$ and $\gamma$ according to $\phi = \rho\mathrm{e}^{\mathrm{i}\gamma}$. The unitarity gauge is recovered by the gauge transformation

$$\mathbf{A} \to \mathbf{A} - \frac{1}{e_B}\nabla\gamma(x) \quad (5)$$

and the original transverse vector field $\mathbf{A}_\perp$ acquires a longitudinal component $\mathbf{A}_L$ proportional to $\nabla\gamma$. Thus the original measure in equation (4) becomes

$$\int D[\phi, \phi^*, \mathbf{A}_\perp] = \int D[\gamma]\rho D[\rho]D[\mathbf{A}_\perp] \to \text{const.} \times \int \rho D[\rho]D[\mathbf{A}_L]D[\mathbf{A}_\perp]. \quad (6)$$

In unitarity gauge the action, equation (1), now reads

$$S = \int \mathrm{d}^3x \left\{\frac{1}{2}(\nabla\rho)^2 + \frac{1}{2}m_B^2\rho^2 + \lambda_B\rho^4 + \frac{1}{2}e_B^2\rho^2(A_L^2 + A_\perp^2) + \frac{1}{2}(\nabla \times \mathbf{A}_\perp)^2\right\} \quad (7)$$

and the longitudinal field $\mathbf{A}_L$ may be integrated out exactly yielding a constant factor and an extra $1/\rho$ factor for the measure (6). Finally, dropping the constant factors, the partition function may be written as

$$Z = \int D[\rho, \mathbf{A}_\perp] \exp\left\{-\int \mathrm{d}^3x \left[\frac{1}{2}(\nabla\rho)^2 + \frac{1}{2}m_B^2\rho^2 + \lambda_B\rho^4 + \frac{1}{2}e_B^2\rho^2A_\perp^2 + \frac{1}{2}(\nabla \times \mathbf{A}_\perp)^2\right]\right\}. \quad (8)$$

We may enforce the transversal condition on the vector field by a gauge fixing term in the action and, restoring $\rho = \phi$, the action reads

$$S = \int \mathrm{d}^3x \left[\frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m_B^2\phi^2 + \lambda_B\phi^4 + \frac{1}{2}e_B^2\phi^2A^2 + \frac{1}{2}(\nabla \times \mathbf{A})^2 + \frac{1}{2\epsilon}(\nabla \cdot \mathbf{A})^2\right]. \quad (9)$$

The partition function is now expressed as a functional integral over the real scalar field $\phi$ and the generic three-dimensional vector field $\mathbf{A}$, with the extra prescription that the parameter $\epsilon$ is set to zero at the end of the calculation. Inserting a source term we may write

$$Z[j] = \int D[\phi, A_\mu] \exp\left\{-S + \int \mathrm{d}^3xj\phi\right\} \quad (10)$$

with $S$ given by equation (9). The free energy (effective potential) follows by the Legendre transformation

$$\mathcal{F}[\varphi] = -\ln Z + \int \mathrm{d}^3xj\varphi \quad (11)$$

where $\varphi$ is the average value of $\phi$ in presence of the source $j$. The superconducting phase is characterized by an absolute minimum of $\mathcal{F}$ for $\varphi \neq 0$.

## 3 The Gaussian method

From the partition function (10), the GEP may be evaluated by the $\delta$ expansion method discussed in references [9,13]. In our case the GEP represents a variational estimate of the free energy (11).

First we introduce a shifted field

$$\tilde{\phi} = \phi - \varphi \tag{12}$$

then we split the Lagrangian into two parts

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{int} \tag{13}$$

where $\mathcal{L}_0$ is the sum of two free-field terms describing a vector field $A_\mu$ with mass $\Delta$ and a real scalar field $\tilde{\phi}$ with mass $\Omega$:

$$\mathcal{L}_0 = \left[+\frac{1}{2}(\nabla \times \mathbf{A})^2 + \frac{1}{2}\Delta^2 A_\mu A^\mu + \frac{1}{2\epsilon}(\nabla \cdot \mathbf{A})^2\right] + \left[\frac{1}{2}(\nabla\tilde{\phi})^2 + \frac{1}{2}\Omega^2\tilde{\phi}^2\right]. \tag{14}$$

The interaction then reads

$$\mathcal{L}_{int} = v_0 + v_1\tilde{\phi} + v_2\tilde{\phi}^2 + v_3\tilde{\phi}^3 + v_4\tilde{\phi}^4 + \frac{1}{2}\left(e_B^2\varphi^2 - \Delta^2\right)A_\mu A^\mu + e_B^2\varphi A_\mu A^\mu\tilde{\phi} + \frac{1}{2}e_B^2 A_\mu A^\mu\tilde{\phi}^2 \tag{15}$$

where

$$v_0 = \frac{1}{2}m_B^2\varphi^2 + \lambda_B\varphi^4 \tag{16a}$$

$$v_1 = m_B^2\varphi + 4\lambda_B\varphi^3 \tag{16b}$$

$$v_2 = \frac{1}{2}m_B^2 + 6\lambda_B\varphi^2 - \frac{1}{2}\Omega^2 \tag{16c}$$

$$v_3 = 4\lambda_B\varphi \tag{16d}$$

$$v_4 = \lambda_B. \tag{16e}$$

We now expand the free energy to first order in $\mathcal{L}_{int}$ following standard perturbation theory procedures. We obtain

$$\mathcal{F}[\varphi] = \frac{1}{2}\operatorname{Tr}\ln\left[g^{-1}(x,y)\right] + \frac{1}{2}\operatorname{Tr}\ln\left[G_{\mu\nu}^{-1}(x,y)\right] + \int \mathrm{d}^3x\Big\{v_0 + v_2 g(x,x) + 3v_4 g^2(x,x) + \frac{1}{2}e_B^2\left(g(x,x) + \varphi^2 - \Delta^2\right)G_{\mu\mu}(x,x)\Big\} \tag{17}$$

where $g(x,y)$ is the free-particle propagator for the scalar field, and $G_{\mu\nu}(x,y)$ is the free-particle propagator for the vector field

$$G_{\mu\nu}^{-1}(x,y) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\Big[\delta_{\mu\nu}(k^2 + \Delta^2) + \left(\frac{1}{\epsilon} - 1\right)k_\mu k_\nu\Big]. \tag{18}$$

In the limit $\epsilon \to 0$, up to an additive constant

$$\operatorname{Tr}\ln\left[G_{\mu\nu}^{-1}(x,y)\right] = 2\mathcal{V}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\ln(k^2 + \Delta^2) \tag{19}$$

where $\mathcal{V}$ is the total volume. Dropping all constant terms, the free energy density $V_{\text{eff}} = \mathcal{F}/\mathcal{V}$ (effective potential) reads

$$V_{\text{eff}}[\varphi] = I_1(\Omega) + 2I_1(\Delta) + \left[\lambda_B\varphi^4 + \frac{1}{2}m_B^2\varphi^2 + \frac{1}{2}\left\{m_B^2 - \Omega^2 + 12\lambda_B\varphi^2 + 6\lambda_B I_0(\Omega)\right\}I_0(\Omega)\right] + \left(e_B^2\varphi^2 + e_B^2 I_0(\Omega) - \Delta^2\right)I_0(\Delta) \tag{20}$$

where the divergent integrals $I_n$ are defined according to

$$I_0(M) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{M^2 + k^2} \tag{21}$$

$$I_1(M) = \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\ln(M^2 + k^2) \tag{22}$$

and are regularized by insertion of a finite cut-off $\Lambda$.

The free energy (20) now depends on the mass parameters $\Omega$ and $\Delta$. Since none of them was present in the original GL action of equation (9), the free energy should not depend on them, and the *minimum sensitivity* method [16] can be adopted in order to fix the masses: the free energy is required to be stationary for variations of $\Omega$ and $\Delta$. On the other hand the stationary point can be shown to be a minimum for the free energy and the method is equivalent to a pure variational method [9]. At the stationary point the masses give the inverse correlation lengths for the fields, the so called coherence length $\xi = 1/\Omega$ and penetration depth $\ell = 1/\Delta$.

The stationary conditions

$$\frac{\partial V_{\text{eff}}}{\partial\Omega^2} = 0 \tag{23a}$$

$$\frac{\partial V_{\text{eff}}}{\partial\Delta^2} = 0 \tag{23b}$$

give two coupled gap equations:

$$\Omega^2 = 12\lambda_B I_0(\Omega) + m_B^2 + 12\lambda_B\varphi^2 + 2e_B^2 I_0(\Delta) \tag{24a}$$

$$\Delta^2 = e_B^2\varphi^2 + e_B^2 I_0(\Omega). \tag{24b}$$

For any $\varphi$ value, equations (24) must be solved numerically, and the minimum point values $\Omega$ and $\Delta$ must be inserted back into equation (20) in order to get the Gaussian free energy $V_{\text{eff}}(\varphi)$ as a function of the order parameter $\varphi$. For a negative and small enough $m_B^2$, we find that $V_{\text{eff}}$ has a minimum at a non zero value of $\varphi = \varphi_{\min} > 0$, thus indicating that the system is in the broken-symmetry superconducting phase. Of course the masses $\Omega$, $\Delta$ only

take their physical value at the minimum of the free energy $\varphi_{\min}$. This point may be found by requiring that

$$\frac{\partial V_{\text{eff}}}{\partial \varphi^2} = 0 \tag{25}$$

where as usual the partial derivative is allowed as far as the gap equations (24) are satisfied [7]. The condition (25) combined with the gap equation (24a) yields the very simple result

$$\varphi^2_{\min} = \frac{\Omega^2}{8\lambda_B}. \tag{26}$$

However we notice that here the mass $\Omega$ must be found by solution of the coupled gap equations. Thus equation (26) and (24) must be regarded as a set of coupled equations and must be solved together in order to find the physical values for the correlation lengths and the order parameter.

Insertion of equation (26) into equation (24b) yields a simple relation for the GL parameter $\kappa_{\text{GL}}$

$$\kappa^2_{\text{GL}} = \left(\frac{\ell}{\xi}\right)^2 = \kappa_0^2 \frac{1}{1 + \dfrac{I_0(\Omega)}{\varphi^2_{\min}}} \tag{27}$$

where $\kappa_0 = e_B^2/(8\lambda_B)$ is the mean-field GL parameter which does not depend on temperature. Equation (27) shows that the GL parameter is predicted to be temperature dependent through the non trivial dependence of $\Omega$ and $\varphi_{\min}$. At low temperature, where the order parameter $\varphi_{\min}$ is large, the deviation from the mean-field value $\kappa_0$ is negligible. Conversely, close to the critical point, where the order parameter is vanishing, the correction factor in equation (27) becomes very important.

## 4 Comparison with experimental data

In order to make contact with the phenomenology of the high-$T_c$ cuprate superconductors we need to fix the bare parameters of the GL action. The standard derivation [15] of the GL action (1) from a microscopic model gives a direct connection between microscopic *first-principle* quantities and phenomenological bare parameters. The bare coupling $e_B$ turns out to be related to the elementary charge of fermions, to the critical temperature $T_c$ and to the zero temperature coherence length $\xi_0$ through [15]

$$e_B = \frac{2e}{\hbar c}\sqrt{k_B T_c \xi_0}. \tag{28}$$

The other parameters may be fixed by knowledge of some zero temperature phenomenological quantities like coherence length and penetration depth. The bare mass parameter $m_B^2$ may be regarded as a linear function of temperature

$$m_B^2 = m_c^2 + \left(1 - \frac{T}{T_c}\right)(m_0^2 - m_c^2) \tag{29}$$

where $m_0^2$ is the value which is required in order to find $\Omega = 1/\xi_0$ from the gap equation (24a) at $\varphi = \varphi_{\min}$, and

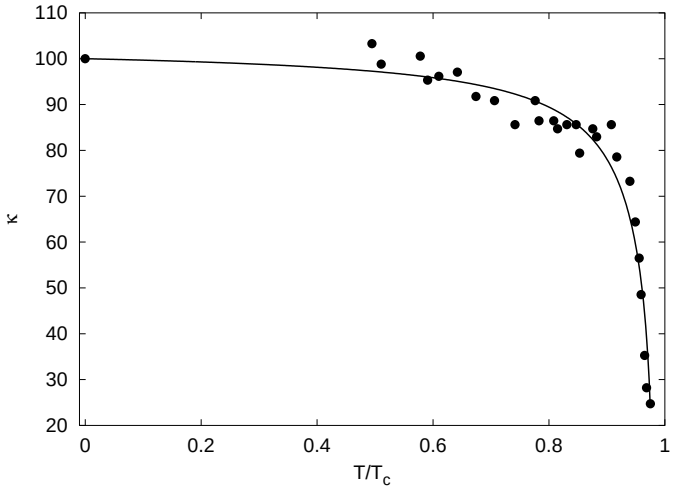


**Fig. 1.** The GL parameter according to equation (27) for $\kappa_0 = 100$, $\xi_0 = 1.36$ nm, $T_c = 121.5$ K and $\Lambda\xi_0 = 57$ (full line). The circles are the experimental data of reference [12] for $Tl_2Ca_2Ba_2Cu_3O_{10}$.

$m_c^2$ is the value of $m_B^2$ at the transition point. In mean-field approximation $m_c^2 = 0$, while here the fluctuations shift the transition point to a non vanishing $m_B^2$ value. The bare coupling $\lambda_B$ is regarded as a constant, and is fixed through equation (24b) by requiring that at zero temperature (*i.e.*, for $m_B^2 = m_0^2$) the penetration depth $\ell_0 = 1/\Delta$. This way the method provides a one-parameter interpolation scheme for the superconducting properties, as the cut-off $\Lambda$ still has to be fixed. The cut-off $\Lambda$ is a characteristic energy scale of the sample, and may be determined by a direct fit of the experimental data.

Unfortunately there are not too many available experimental data on the behaviour of superconductors close to the critical point. Even for the high-$T_c$ cuprate superconductors the measurement of both coherence length and penetration depth up to the pre-critical region is not an easy task. The GL parameter has been reported by Brandstatter *et al.* [12] as a function of temperature for the high $T_c$ material $Tl_2Ca_2Ba_2Cu_3O_{10}$ ($T_c = 121.5$ K, $\kappa_0 = 100$, $\xi_0 = 1.36$ nm). These data are shown in Figure 1 together with the interpolation curve obtained by equation (27) for $\Lambda\xi_0 = 57$. We observe that the experimental GL parameter is almost constant $\kappa_{\text{GL}} \approx \kappa_0$ up to $T = 0.8T_c$ where it starts decreasing. Thus for $T/T_c > 0.8$ the mean-field approximation breaks down and the thermal fluctuations become important. On the other hand equation (27) fits the experimental data up to 98% of the critical temperature. Beyond that point there are neither experimental data nor reliable theoretical predictions. As we approach the critical point some universal behaviour should be expected and the role of thermal fluctuations becomes too important to be dealt with by the present method [17].

In perturbative calculations, at one-loop order, the unitarity gauge is known [18] to give rise to wrong predictions around the critical point. Thus it could be argued that, because of the bad ultraviolet behaviour of the gauge propagator, higher order diagrams should be included to

cancel the divergences even in the present one loop calculation. However, at variance with perturbative approximations, variational calculations are known to be less sensitive to higher order corrections. The GEP provides very sensible results even when the one loop effective potential fails entirely [7]. Moreover, while the way of dealing with divergences is crucial at the critical point, the present calculation deals with a pre-critical region where the cut-off regulator is finite and plays the role of a physical length scale which is naturally determined by the structure of the condensed matter system. Thus divergences are not an issue: our unitarity gauge Lagrangian must be regarded as regularized and is known [18] to give the same results predicted by other gauge choices.

It must be kept in mind that all variational methods are quite sensitive to the choice of the trial functional. The Gaussian functional is not by itself gauge invariant, and a gauge dependent result is expected anyway by this variational method. The question of determining the best gauge choice has been addressed by Ibañez-Meier *et al.* [9] who found the Landau gauge $(\partial \cdot A) = 0$ to be optimal in four dimensions by variational arguments. In three dimensions that is equivalent to the transverse gauge we started with in Section 2. Unfortunately the Gaussian functional also breaks the $U(1)$ symmetry of the Lagrangian, and unphysical massive degrees of freedom show up unless the unitarity gauge is chosen. Thus our gauge prescription must be regarded as a compromise which allows to make contact with the real phenomenology. The comparison with experimental data is encouraging in this respect.

As the GEP provides a nice way to interpolate the experimental data beyond the mean-field regime, we expect the method to be reliable for the description of symmetry breaking in $3 + 1$ dimensions where the scalar electrodynamics may be regarded as a toy model for the standard electro-weak theory. Since there is no reason to believe that the real universe is very close to the transition point, the Gaussian method may be regarded as a valid tool for describing the effects of fluctuations beyond mean-field approximation.

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