A minimal size for granular superconductors

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(November 19, 2018)

Abstract We investigate the minimal size of small superconducting grains by means of a Ginzburg-Landau model confined to a sphere of radius $R$. This model is supposed to describe a material in the form of a ball, whose transition temperature when presented in bulk form, $T_0$, is known. We obtain an equation for the critical temperature as a function of $R$ and of $T_0$, allowing us to arrive at the minimal radius of the sphere below which no superconducting transition exists.

PACS Number(s): 11.10.-z, 74.20.-z, 74.81.Bd

I. INTRODUCTION

Recently, experimental results on small metallic grains [1] led to an important effort on theoretical investigations of superconducting pairing correlations in nanograins [2]. Many of the present developments in this area are based on the exact solution of the discrete BCS model [3]. This model is described by a Hamiltonian for a discrete set of doubly-degenerate energy levels containing a pairing interaction for the scattering of pairs of electrons at levels next to each other. One of the fundamental questions addressed by these works has been stated long ago [4] and was restated in the following form [1]: What is the lower size limit for the existence of superconductivity in small grains?

In the present letter we present an answer for the above question from another point of view, stemming from the field theory framework of the Ginzburg-Landau model. Our approach consists in considering an Euclidean massive ($\lambda \phi^4$) model describing a system constrained to be confined to a sphere of radius $R$. The rationale for our procedure is twofold, on one hand the Ginzburg-Landau model provides a well established and elegant theory of the phenomenology of the superconducting state. On the other hand, for Euclidean field theories, temperature, understood as imaginary time, and spatial coordinates share the same footing, which allows us to apply to the spatial coordinates a compactification mechanism using the Matsubara formalism [5–7]. We emphasize that we are considering an Euclidean field theory in $D$ purely spatial dimensions, so we are not working in the framework of finite temperature field theory. Here, temperature is introduced in the mass term of the Hamiltonian (1.1) below by means of the usual Ginzburg-Landau prescription.

We must stress here that we do not pretend to attain the degree of understanding coming from microscopic theories like BCS [8] or the reduced BCS [3], nevertheless we believe that our perspective can shed some light on this interesting question.

We consider the Ginzburg-Landau Hamiltonian density,

$$\mathcal{H} = \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} m_0^2 \phi^2 + \frac{u}{4!} \phi^4,$$  \hspace{1cm} (1.1)

in Euclidean 3-dimensional space, where $u$ is the coupling constant, and $m_0^2 = \alpha (T - T_0)$ is the squared bare mass ($T_0$ being the bulk transition temperature of the superconductor and $\alpha > 0$). From a physical point of view, introducing temperature by means of the mass term in this Hamiltonian (1.1) below should correspond to a spherical sample of material. We investigate the behaviour of the system as a function of the radius $R$ of the confining sphere, in the approximation in which gauge fluctuations are neglected, and using spherical coordinates. Under these conditions one can write the generating functional of the correlation functions as

$$Z = \int \mathcal{D} \phi \mathcal{D} \phi^* exp \left( - \int_0^R dr \int d\Omega \mathcal{H} (\phi, \nabla \phi) \right),$$  \hspace{1cm} (1.2)

with the field $\phi(r, \theta, \phi)$ satisfying the condition of confinement along the r-axis, $\phi(r = 0) = \phi(r = R) = 0$. These conditions of confinement of the r-dependence of the field to a sphere of radius $R$, permit us to proceed with respect to the r-coordinate, in a manner analogous as it is done in the imaginary-time Matsubara formalism in field theory. The Feynman rules should be modified following the prescription,
\begin{equation}
\int \frac{dk_r}{2\pi} \to \frac{1}{R} \sum_{n=-\infty}^{+\infty} \quad k_r \to \frac{2n\pi}{R} \equiv \omega_n.
\end{equation}

The letter is organized as follows. In the next section we calculate the compactified effective potential obtaining its \(R\)-dependence. The suppression of superconductivity as a function of the grain radius is shown in section 3. Section 4 present some concluding remarks.

**II. THE \(R\)-DEPENDENT EFFECTIVE POTENTIAL**

We start from the expression for the one-loop contribution to the effective potential in absence of boundaries in spherical coordinates \(U_1(\phi_0, R = \infty)\), where in order to deal with dimensionless quantities in the required regularization procedures, we introduce parameters \(c^2 = m^2/4\pi^2\mu^2\), \((R\mu)^2 = a^{-1}\), \(g = (u/8\pi^2)\), \((\varphi_0/\mu) = \phi_0\), \(\varphi_0\) being the normalized vacuum expectation value of the field (the classical field) and \(\mu\) a mass scale. In terms of these parameters,

\begin{equation}
U_1(\phi_0, R = \infty) = \mu^3 \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} g^s \phi_0^{2s} \int d\Omega \frac{k_2 dk_r}{(k_r^2 + c^2)^s},
\end{equation}

here \(m\) is the renormalized mass and the integration over the solid angle \(d\Omega\) gives simply a factor \(4\pi\). Performing the replacements defined in (1.3), we obtain the boundary-dependent (\(R\)-dependent) one-loop contribution to the effective potential in the form,

\begin{equation}
U_1(\phi_0, R) = 4\pi \mu^3 a^{3/2} \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} g^s \phi_0^{2s} \times
\end{equation}

\begin{equation}
\times \sum_{n=-\infty}^{+\infty} \frac{n^2}{(an^2 + c^2)^s}.
\end{equation}

This equation can be rewritten using the property

\begin{equation}
\sum_{n=-\infty}^{+\infty} \frac{n^2}{(an^2 + c^2)^s} = \frac{-1}{s-1} \frac{d}{da} A^2_1 (s-1; a),
\end{equation}

where \(A^2_1 (s-1; a)\) is one of the Epstein-Hurwitz \(\zeta\)-functions [9] defined by,

\begin{equation}
A^2_1 (\nu; a_1, \ldots, a_d) = \sum_{\{n_i\} = -\infty}^{+\infty} \frac{1}{(a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^\nu},
\end{equation}

valid for \(\text{Re}(\nu) > d/2\) (in our case \(\text{Re}(s) > 1/2\)). Then Eq.(2.2) becomes,

\begin{equation}
U_1(\phi_0, R) = -4\pi \mu^3 a^{3/2} \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s(s-1)} g^s \phi_0^{2s} \times
\end{equation}

\begin{equation}
\times \frac{d}{da} A^2_1 (s-1; a).
\end{equation}

The Epstein-Hurwitz \(\zeta\)-function can be extended to the whole complex \(s\)-plane generalizing as is done in [5] the mode sum regularization procedure described in Ref. [9]. We write,

\begin{equation}
A^2_1 (\nu; a_1, \ldots, a_d) = \frac{1}{c^{2\nu}} + 2 \sum_{i=1}^{d} \sum_{n_i=1}^{\infty} (a_i n_i^2 + c^2)^{-\nu} +
\end{equation}

\begin{equation}
2^2 \sum_{i<j=1}^{d} \sum_{n_i,n_j=1}^{\infty} (a_i n_i^2 + a_j n_j^2 + c^2)^{-\nu} + \cdots
\end{equation}

\begin{equation}
+ 2^d \sum_{n_1, \ldots, n_d=1}^{\infty} (a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^{-\nu}.
\end{equation}
Using the identity,

\[
\frac{1}{\Delta^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty dt \, t^{\nu-1} e^{-\Delta t},
\]
we get,

\[
A_{\delta}^2(\nu; a_1, \ldots, a_d) = \frac{1}{\Gamma(\nu)} \int_0^\infty dt \, t^{\nu-1} e^{-c^2 t} \left[ 1 + 2 \sum_{i=1}^d T_1(t, a_i) + 
+ 2^2 \sum_{i,j=1}^d T_2(t, a_i, a_j) + \cdots + 2^d T_d(t, a_1, \ldots, a_d) \right],
\]

where,

\[
T_1(t, a_i) = \sum_{n_i=1}^\infty e^{-a_i n_i^2 t},
\]

\[
T_j(t, a_1, \ldots, a_j) = T_j-1(t, a_1, \ldots, a_{j-1}) T_1(t, a_j), \quad j = 2, \ldots, d.
\]

Considering the property of functions \( T_1 \),

\[
T_1(t, a_i) = \frac{1}{2} + \sqrt{\frac{\pi}{a_i t}} \left[ \frac{1}{2} + S\left(\frac{\pi^2}{a_i t}\right) \right],
\]

where

\[
S(x) = \sum_{n=1}^\infty e^{-n^2 x},
\]
we can notice that the surviving terms in Eq.(2.6) are proportional to \((a_1 \cdots a_d)^{-1/2}\). Therefore we find,

\[
A_{\delta}^2(\nu; a_1, \ldots, a_d) = \frac{\pi^{\nu}}{\sqrt{a_1 \cdots a_d} \Gamma(\nu)} \int_0^\infty dt \, t^{\nu\frac{1}{2}+1} e^{-c^2 t} \left[ 1 + 2 \sum_{i=1}^d S\left(\frac{\pi^2}{a_i t}\right) + 2^2 \sum_{i<j=1}^d S\left(\frac{\pi^2}{a_i t}\right) S\left(\frac{\pi^2}{a_j t}\right) + \cdots + 2^d \prod_{i=1}^d S\left(\frac{\pi^2}{a_i t}\right) \right].
\]

Inserting in Eq.(2.13) the explicit form of the function \( S(x) \) in Eq.(2.12) and using the following representation for Bessel functions of the third kind, \( K_{\nu} \),

\[
2(a/b)^{\nu} K_{\nu}(2\sqrt{ab}) = \int_0^\infty dx \, x^{\nu-1} e^{-(a/x)-bx},
\]
we obtain after some long but straightforward manipulations,

\[
A_{\delta}^2(\nu; a_1, \ldots, a_d) = \frac{2^{\nu-\frac{1}{2}} \Gamma(\nu - \frac{d}{2})}{\Gamma(\nu)} \left[ 2^{\nu-\frac{1}{2}} e^{-\Delta t} \right] \left[ 1 + \sum_{i=1}^d \left( \frac{m}{L_i n_i} \right)^{\nu-\frac{d}{2}} K_{\nu-\frac{d}{2}}(m L_i n_i) + \cdots + 2^d \prod_{i=1}^d \left( \frac{m}{L_i n_i} \right)^{\nu-\frac{d}{2}} \times K_{\nu-\frac{d}{2}}(m \sqrt{L_i^2 n_i^2 + \cdots + L_d^2 n_d^2}) \right].
\]
For $d = 1$, taking $\nu = s - 1$, and identifying the compactified dimension with the radial coordinate, we obtain in our case from Eq.(2.5) the one-loop correction to the effective potential,

$$U_1(\phi_0, R) = -4\pi \mu^3 a^{3/2} \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s(s-1)} g^s \phi_0^{2s} 2^{s-1/2} \frac{\pi^{2s-5/2}}{\Gamma(s-1)} \times$$

$$\times \frac{d}{da} \left( \frac{1}{\sqrt{a}} \right) \left[ 2^{s-5/2} \Gamma(s-\frac{3}{2}) \frac{m}{\mu}^3 2s + 2 \sum_{n=1}^{\infty} \left( \frac{m}{nR} \right)^{\frac{1}{2}} K_{s-\frac{1}{2}}(mnR) \right],$$

or, remembering $a^{-1} = (R\mu)^2$ and $\phi_0 = \varphi_0/\mu$,

$$U_1(\varphi_0, R) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{s!} 2^{s+1/2} \pi^{2s-3/2} g^s \varphi_0^{2s} \times$$

$$\times \left[ 2^{s-7/2} \Gamma(s-\frac{3}{2}) \frac{m}{\mu}^3 2s + 2 \sum_{n=1}^{\infty} \left( \frac{m}{nR} \right)^{\frac{1}{2}} K_{s-\frac{1}{2}}(mnR) \right] + R \frac{d}{dR} \sum_{n=1}^{\infty} \left( \frac{m}{nR} \right)^{\frac{1}{2}} K_{s+\frac{1}{2}}(mnR).$$

(2.16)

where $K_{s+\frac{1}{2}}$ are Bessel functions of the third kind.

### III. CRITICAL BEHAVIOUR

As we are analyzing the case where the field has only one component we can neglect the $R$-dependence of the coupling constant, that is we consider $u$ as the renormalized coupling constant. In this case, it is enough for us to use only one renormalization condition,

$$\frac{\partial^2}{\partial \varphi_0^2} U_1(\varphi_0, R) |_{\varphi_0=0} = m^2.$$  

(3.1)

Notice that we are using a modified minimal subtraction scheme [10], where the mass (and coupling constant, if it is the case) counter-terms are for even space dimension $D$, poles of Gamma-functions at the physical values of $s$ ($s = 1$ for the mass, $s = 2$ for the coupling constant). For arbitrary $D$, we would have in the $R$-independent term in Eq.(2.17), instead of the factor $\Gamma(s-\frac{1}{2})$, a factor $\Gamma(s-\frac{D}{2})$, which would generate a pole at $s = 1$ for even dimensions. This polar term should be subtracted, giving the $R$-dependent correction to the renormalized mass proportional to the regular part of the analytical extension of the Epstein-Hurwitz zeta-function in the neighbourhood of the pole at $s = 1$. For odd space dimensions, as for our case $D = 3$, there are no poles of Gamma-functions, but in order to have a coherent procedure in any dimension, we also subtract the corresponding term, performing a finite renormalization. Thus the $R$-dependent renormalized mass, at one-loop approximation, is given by

$$m^2(R) = m_0^2 + \frac{u}{3\sqrt{2\pi}^{3/2}} \left[ \sum_{n=1}^{\infty} \left( \frac{m_0}{nR} \right)^{1/2} K_{s+\frac{1}{2}}(nRm_0) \right] +$$

$$+ R \frac{d}{dR} \sum_{n=1}^{\infty} \left( \frac{m_0}{nR} \right)^{1/2} K_{s-\frac{1}{2}}(nRm_0).$$

(3.2)

On the other hand, if we start in the ordered phase, the model exhibits spontaneous symmetry breaking, but for sufficiently small values of $T^{-1}$ and $R$ the symmetry is restored. We can define the critical curve $C(T, R)$ as the curve in the $T \times R$ plane for which the inverse squared correlation length, $\xi^{-2}(T, R, \varphi_0)$, vanishes in the $R$-dependent gap equation,

$$\xi^{-2} = m_0^2 + u \varphi_0^2 +$$

$$+ \frac{u}{6R} \sum_{n=-\infty}^{\infty} \int \frac{d\Omega}{(2\pi)^2} \frac{\omega_n^2}{\omega_n^2 + \xi^{-2}},$$

(3.3)
where \( \phi_0 \) is the normalized vacuum expectation value of the field (different from zero in the ordered phase). In the disordered phase, in particular in the neighborhood of the critical curve, \( \phi_0 \) vanishes and the gap equation reduces to a \( R \)-dependent Dyson-Schwinger equation,

\[
m^2(T, R) = m_0^2(T) + \frac{u}{6R} \times \sum_{n=-\infty}^{\infty} \int \frac{d\Omega}{(2\pi)^2} \frac{\omega^2}{\omega_n^2 + m^2(T, R)}.
\]

After steps analogous to those leading from Eq.(2.2) to Eq.(3.2), Eq.(3.4) can be written in the form

\[
m^2(T, R) = m_0^2 + \frac{u}{3\sqrt{2}\pi^{3/2}} \times \\
\times \left[ \sum_{n=1}^{\infty} \left( \frac{m(T, R)}{nR} \right)^{1/2} K_{\frac{1}{2}}(nRm(T, R)) \right] + \\
+ R \frac{d}{dR} \sum_{n=1}^{\infty} \left( \frac{m(T, R)}{nR} \right)^{1/2} K_{\frac{1}{2}}(nRm(T, R))
\]

(3.5)

If we limit ourselves to the neighborhood of criticality, \( m^2(T, R) \approx 0 \), we may investigate the behavior of the system by using in Eq.(3.5) an asymptotic formula for small values of the argument of Bessel functions,

\[
K_{\nu}(z) \approx \frac{1}{2} \Gamma(\nu) \left( \frac{z}{2} \right)^{\nu} (z \sim 0).
\]

(3.6)

Performing the derivative in Eq.(3.5) with the help of the formula,

\[
\frac{d}{dz} K_{\nu}(z) = vz^{-1} K_{\nu}(z) - K_{\nu+1}(z),
\]

(3.7)

and using the tabulated values \( \Gamma(1/2) = \sqrt{\pi}, \Gamma(3/2) = \sqrt{\pi}/2 \), we obtain after some manipulations in the neighbourhood of criticality,

\[
m^2(T, R) \approx m_0^2 + \frac{u\zeta(1)}{6\pi R},
\]

(3.8)

where \( \zeta(z) \) is the Riemann \textit{zeta}-function defined for \( z > 1 \).

Eq.(3.8) is of course meaningless as it stands. In order to obtain a critical curve and give a meaning to eq.(3.8), we perform an analytic continuation of the \textit{zeta}-function \( \zeta(z) \) to values of the argument \( z \leq 1 \), by means of its reflection property,

\[
\zeta(z) = \frac{1}{\Gamma(z/2)} \Gamma\left(\frac{1-z}{2}\right) \pi^{\frac{1}{2}-\frac{z}{2}} \zeta(1-z),
\]

(3.9)

which defines a meromorphic function having only one simple pole at \( z = 1 \). The physical interpretation is achieved through a mass renormalization procedure that can be done as follows: remembering the formula

\[
\lim_{z \to 1} \left[ \zeta(z) - \frac{1}{1-z} \right] = \gamma,
\]

(3.10)

where \( \gamma \approx 0.57216 \) is the Euler constant, the \textit{renormalized} mass \( \bar{m} \) is then defined as

\[
\bar{m}^2(T, R) = \lim_{z \to 1} \left[ m^2(T, R) - \frac{u}{6\pi R(z - 1)} \right] = \alpha(T - T_0) + \frac{u\gamma}{6\pi R}.
\]

(3.11)

Taking this \textit{renormalized} mass equal to zero leads to the critical temperature, given as a function of the radius \( R \) by,
\[ T_c = T_0 - \frac{u \gamma}{6\pi R}. \]  

(3.12)

In Eq. (3.12), \( T_0 \) corresponds to the transition temperature for the material in absence of boundaries \( (R \to \infty) \), that is, to the bulk transition temperature. We see then that, in a spherical sample made of the same material, the critical temperature is diminished by a quantity proportional to the inverse of its radius. Also, we see that there is a minimal radius \( R^{(0)} \) below which superconductivity is suppressed. Identifying the usual 3-dimensional Ginzburg-Landau parameter \( \beta = u \), the minimal radius is given by,

\[ R^{(0)} = \frac{\gamma \beta}{6\pi \alpha T_0}. \]  

(3.13)

IV. CONCLUDING REMARKS

In this letter, within the framework of the Ginzburg-Landau model, we were able to describe a spherical system, a grain, and we showed that, below a specific size, superconductivity is suppressed. Our method made use of effective potential and dimensional renormalization techniques supplemented by the Matsubara prescription (1.3) which give us a structure to work in a spherical geometry. We did not attempt to deal with the microscopic properties of ultrasmall metallic grains, however we believe that our approach can pave the way to further studies of the superconducting state in different geometries, notably through Monte Carlo and variational techniques.

V. ACKNOWLEDGEMENTS

This work has been supported by the Brazilian agency CNPq (Brazilian National Research Council). One of us, IR, also thank Pronex/MCT for partial support.

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