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Critical temperature for first-order phase transitions in confined systems

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Abstract. We consider the Euclidean D-dimensional $-\lambda|\varphi|^4 + \eta|\varphi|^6$ $(\lambda, \eta > 0)$ model with d $(d \leq D)$ compactified dimensions. Introducing temperature by means of the Ginzburg–Landau prescription in the mass term of the Hamiltonian, this model can be interpreted as describing a first-order phase transition for a system in a region of the D-dimensional space, limited by d pairs of parallel planes, orthogonal to the coordinates axis x_1, x_2, ..., x_d. The planes in each pair are separated by distances L_1, L_2, ..., L_d. We obtain an expression for the transition temperature as a function of the size of the system, $T_c(\{L_i\})$, $i = 1, 2, \ldots, d$. For $D = 3$ we particularize this formula, taking $L_1 = L_2 = \cdots = L_d = L$ for the physically interesting cases $d = 1$ (a film), $d = 2$ (an infinitely long wire having a square cross-section), and for $d = 3$ (a cube). For completeness, the corresponding formulas for second-order transitions are also presented. Comparison with experimental data for superconducting films and wires shows qualitative agreement with our theoretical expressions.

PACS. 03.70.+k Theory of quantized fields – 11.10.-z Field theory

1 Introduction

Studies on field theory applied to second-order phase transitions have been done in the literature for a long time. A thorough account on the subject can be found in references [1–7]. Under the assumption that information about general features of the behavior of systems undergoing phase transitions can be obtained in the approximation which neglects gauge field contributions in the Ginzburg–Landau model, investigations have been done with an approach different from the renormalization-group analysis. The system confined between two parallel planes has been considered and using the formalism developed in reference [8] the way in which the critical temperature for a second-order phase transition is affected by the presence of confining boundaries has been investigated. In particular, a study has been carried out on how the critical temperature of a superconducting film depends on its thickness [9]. Moreover, confined systems in regions of three-dimensional space with some other shapes were also considered: grains and wires [10,11]. In all those cases a minimal size of these regions can be determined for which the transition is still sustained.

In a previous article [13] we have done a further step, by considering in the simpler case of the system confined between two parallel planes, the model which besides the quartic scalar field self-interaction, a sextic one is also present. The model with both interactions taken together leads to a renormalizable quantum field theory in three dimensions and, in the context considered in reference [13], it describes *first-order* phase transitions in films. In this paper we extend this formalism to a general framework, considering the Euclidean D-dimensional $-\lambda|\varphi|^4 + \eta|\varphi|^6$ $(\lambda, \eta > 0)$model with d $(d \leq D)$ compactified dimensions, from which we obtain general formulas for the dependence of the transition temperature on the parameters delimiting the spatial region within which the system is confined. Particularizing for $D = 3$, we then consider the superconducting material in the form of a film $(d = 1)$, of a wire $(d = 2)$, and of a grain $(d = 3)$. We also present for comparison the corresponding formulas for second-order transitions.

The usual Ginzburg–Landau Hamiltonian considers only the term $\lambda\varphi^4$ $(\lambda > 0)$. This model is known to lead to second-order phase transitions. But a potential of the type $-\lambda\varphi^4+\eta\varphi^6$ $(\lambda, \eta > 0)$ *ensures* that the system undergoes a *first-order* transition. See, for example, [12]. In some of our previous papers (Refs. [9,11,10]) the $\lambda\varphi^4$ model has been used to determine a theoretical $T_c(L) \times L$ curve for films

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wires and grains and a comparison to experimental data for superconducting films has been done. In the present work we wished to do the same with the extended model in order to compare expected results from second- and first-order transitions. Of course, there are many other potentials that engender first-order transitions, for instance, the Halperin–Lubensky–Ma potential [14], which induces first-order transitions in superconducting materials by effect of integration over the gauge field and takes the form $-\alpha\varphi^3+\beta\varphi^4$. Our potential $-\lambda\varphi^4+\eta\varphi^6$ (λ, $\eta>0$) is just a simple choice to generate first-order transitions in the context of the Ginzburg-Landau theory.

We consider, as in previous publications, that the system is a portion of material of some size, the behavior of which in the critical region is to be derived from a quantum field theory calculation of the dependence of the physical mass parameter on its size. We start from the effective potential, which is related to the physical mass through a renormalization condition. This condition, however, reduces considerably the number of relevant Feynman diagrams contributing to the mass, if one wishes to be restricted to first-order terms in both coupling constants. In fact, just two diagrams need to be considered in this approximation: a tadpole graph with the φ^4 coupling (1 loop) and a "shoestring" graph with the φ^6 coupling (2 loops). No diagram with both couplings occurs. The size-dependence appears from the treatment of the loop integrals. The dimensions of finite extent are treated in momentum space using the formalism of reference [8].

It is worth to notice that for superconducting films with thickness L, a qualitative agreement of our theoretical L-dependent critical temperature is found with experiments. This occurs in particular for thin films (in the case of first-order transitions) and for a wide range of values of L for second-order transitions [13]. Moreover, the recently available experimental data for superconducting wires [22,23] are compatible with our theoretical prediction of the first-order critical temperature as a function of the transverse cross section of the wire.

The paper is organized as follows: In Section 2 we present the model and the general description of the D-dimensional Euclidean system with a compactified d-dimensional subspace; for this, we make an adaptation of the Matsubara formalism suited for our purposes. The contributions from the relevant Feynman diagrams to the effective potential are then established. Next, in Section 3, we exhibit expressions showing the size dependence of the critical temperature for various shapes of confined materials. Comparisons with experimental data for films and wires are shown. Finally, in the the last section we present our conclusions.

2 Effective potential with compactification of a d-dimensional subspace

We consider the scalar field model described by the Ginzburg–Landau Hamiltonian density in a Euclidean D-dimensional space, including both φ^4 and φ^6 interactions, in the absence of external fields, given by (in natural units, $\hbar=c=k_B=1$),

$$\mathcal{H}=\frac{1}{2}\left|\partial_\mu\varphi\right|\left|\partial^\mu\varphi\right|+\frac{1}{2}m_0^2\left|\varphi\right|^2-\frac{\lambda}{4}\left|\varphi\right|^4+\frac{\eta}{6}\left|\varphi\right|^6, \quad (1)$$

where $\lambda>0$ and $\eta>0$ are the *renormalized* quartic and sextic self-coupling constants. Near criticality, the bare mass is given by $m_0^2=\alpha(T/T_0-1)$, with $\alpha>0$ and T_0 being a parameter with the dimension of temperature. Recall that the critical temperature for a first-order transition described by the Hamiltonian above is higher than T_0 [12]. This will be explicitly stated in equation (19) below. Our purpose will be to develop the general case of compactifying a d-dimensional subspace.

We thus consider the system in D dimensions confined to a region of space delimited by $d\leq D$ pairs of parallel planes. Each plane of a pair j is at a distance L_j from the other member of the pair, $j=1,2,\ldots,d$, and is orthogonal to all other planes belonging to distinct pairs $\{i\}$, $i\neq j$. This may be pictured as a parallelepipedal box embedded in the D -dimensional space, whose parallel faces are separated by distances $L_1,L_2,\ldots,L_d$. We use Cartesian coordinates $\mathbf{r}=(x_1,...,x_d,\mathbf{z})$, where $\mathbf{z}$ is a $(D-d)$-dimensional vector, with corresponding momentum $\mathbf{k}=(k_1,...,k_d,\mathbf{q})$, $\mathbf{q}$ being a $(D-d)$-dimensional vector in momentum space. The generating functional of Schwinger functions is written in the form

$$Z=\int\mathcal{D}\varphi\,\mathcal{D}\varphi^*\exp\left(-\int_0^{L_1}dx_1\cdots\int_0^{L_d}dx_d\int d^{D-d}x\,\mathcal{H}(|\varphi|,|\nabla\varphi|)\right), \quad (2)$$

with the field $\varphi(x_1,...,x_d,\mathbf{z})$ satisfying the condition of confinement inside the box, $\varphi(x_i\leq 0,\mathbf{z})=\varphi(x_i\geq 0,\mathbf{z})=$ const. Then, following the procedure developed in reference [8], we are allowed to introduce a generalized Matsubara prescription, performing the following multiple replacements (compactification of a d-dimensional subspace),

$$\int\frac{dk_i}{2\pi}\to\frac{1}{L_i}\sum_{n_i=-\infty}^{+\infty};\qquad k_i\to\frac{2n_i\pi}{L_i},\quad i=1,2...,d. \quad (3)$$

Notice that compactification can be implemented in different ways, as for instance by imposing specific conditions on the fields at spatial boundaries. We here choose periodic boundary conditions.

We emphasize, however, that we are considering a Euclidean field theory in D *purely* spatial dimensions. Therefore, we are *not* working within the framework of finite-temperature field theory. Here, the temperature is introduced in the mass term of the Hamiltonian by means of the usual Ginzburg–Landau prescription.

In principle, the effective potential for systems with spontaneous symmetry breaking is obtained, following the analysis introduced in reference [15], as an expansion in the number of loops in Feynman diagrams. Accordingly, to the free propagator and to the no-loop (tree) diagrams for

both couplings, radiative corrections are added, with increasing number of loops. Thus, at the 1-loop approximation, we get the infinite series of 1-loop diagrams with all numbers of insertions of the φ^4 vertex (two external legs in each vertex), plus the infinite series of 1-loop diagrams with all numbers of insertions of the φ^6 vertex (four external legs in each vertex), plus the infinite series of 1-loop diagrams with all kinds of mixed numbers of insertions of φ^4 and φ^6 vertices. Analogously, we should include all those types of insertions in diagrams with 2 loops, etc. However, instead of undertaking this computation, in our approximation we restrict ourselves to the lowest terms in the loop expansion. We recall that the gap equation we are seeking is given by the renormalization condition in which the physical squared mass is defined as the second derivative of the effective potential $U(\varphi_0)$ with respect to the classical field φ_0, taken at zero field,

$$\left.\frac{\partial^2 U(\varphi_0)}{\partial|\varphi_0|^2}\right|_{\varphi_0=0} = m^2. \tag{4}$$

Within our approximation, we do not need to take into account the renormalization conditions for the interaction coupling constants, i.e., they may be considered as already renormalized when they are written in the Hamiltonian.

At the 1-loop approximation, the contribution of loops with only $|\varphi_0|^4$ vertices to the effective potential is obtained directly from [8], as an adaptation of the Coleman–Weinberg expression after compactification in d dimensions. In this case, we start from the well-known expression for the one-loop contribution to the zero-temperature effective potential in unbounded space [8],

$$U_1(\varphi_0) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s}\left[\frac{\lambda|\varphi_0|^2}{2}\right]^s \int \frac{d^D k}{(k^2+m^2)^s}, \tag{5}$$

where m is the *physical* mass.

In the following, to deal with dimensionless quantities in the regularization procedures, we introduce parameters $c^2 = m^2/4\pi^2\mu^2$, $(L_i\mu)^2 = a_i^{-1}$, $g_1 = (-\lambda/16\pi^2\mu^{4-D})$, $|\varphi_0/\mu^{D-2}|^2 = |\varphi_0|^2$, where φ_0 is the normalized vacuum expectation value of the field (the classical field) and μ is a mass scale. In terms of these parameters and performing the Matsubara replacements (3), the one-loop contribution to the effective potential can be written in the form

$$U_1(\varphi_0, a_1, ..., a_d) = \mu^D\sqrt{a_1\cdots a_d}\sum_{s=1}^{\infty}\frac{(-1)^{s+1}}{2s}g_1^s|\varphi_0|^{2s} \times \sum_{n_1,...,n_d=-\infty}^{+\infty}\int\frac{d^{D-d}q}{(a_1n_1^2+\cdots+a_dn_d^2+c^2+\mathbf{q}^2)^s}. \tag{6}$$

The parameter s counts the number of vertices on the loop.

It is easily seen that only the $s = 1$ term contributes to the renormalization condition (4). It corresponds to the tadpole diagram. It is then also clear that all $|\varphi_0|^6$-vertex and mixed $|\varphi_0|^4$- and $|\varphi_0|^6$-vertex insertions on the 1-loop diagrams do not contribute when one computes the second derivative of similar expressions with respect to the field at zero field: only diagrams with two external legs should survive. This is impossible for a $|\varphi_0|^6$-vertex insertion at the 1-loop approximation. Therefore, the first contribution from the $|\varphi_0|^6$ coupling must come from a higher-order term in the loop expansion. Two-loop diagrams with two external legs and only $|\varphi_0|^4$ vertices are of second order in its coupling constant, and we neglect them, as well as all possible diagrams with vertices of mixed type. However, the 2-loop shoestring diagram, with only one $|\varphi_0|^6$ vertex and two external legs is a first-order (in η) contribution to the effective potential, according to our approximation.

In short, we consider the physical mass as defined at first-order in both coupling constants, by the contributions of radiative corrections from only two diagrams: the tadpole and the shoestring diagrams.

The tadpole contribution reads (putting $s = 1$ in Eq. (6))

$$U_1(\varphi_0, a_1, ..., a_d) = \mu^D\sqrt{a_1\cdots a_d}\,\frac{1}{2}\,g_1|\varphi_0|^2 \times \sum_{n_1,...,n_d=-\infty}^{+\infty}\int\frac{d^{D-d}q}{\mathbf{q}^2+a_1n_1^2+\cdots+a_dn_d^2+c^2}. \tag{7}$$

The integral over the $D-d$ noncompactified momentum variables is performed using the well-known dimensional regularization formula [7]

$$\int\frac{d^l q}{\mathbf{q}^2+M} = \frac{\Gamma(1-\frac{l}{2})\pi^{l/2}}{M^{1-l/2}}; \tag{8}$$

for $l = D-d$, we obtain

$$U_1(\varphi_0, a_1, ..., a_d) = \mu^D\sqrt{a_1\cdots a_d}\sum_{s=1}^{\infty}f(D,d)g_1|\varphi_0|^2Z_d^{c^2} \times\left(\frac{2-D+d}{2}; a_1, ..., a_d\right), \tag{9}$$

where

$$f(D,d) = \pi^{(D-d)/2}\frac{1}{2}\Gamma\left(1-\frac{D-d}{2}\right) \tag{10}$$

and $Z_d^{c^2}(\nu; a_1, ..., a_d)$ are Epstein–Hurwitz zeta-functions, valid for $\mathrm{Re}(\nu) > d/2$, defined by

$$Z_d^{c^2}(\nu; a_1, ..., a_d) = \sum_{n_1,...,n_d=-\infty}^{+\infty}(a_1n_1^2+\cdots+a_dn_d^2+c^2)^{-\nu}. \tag{11}$$

Next, we can proceed to generalizing to several dimensions the mode-sum regularization prescription described in reference [16]. This has been done in reference [8] and it results that the multidimensional Epstein–Hurwitz function has an analytic extension to the whole ν complex plane. In terms of this extended Epstein–Hurwitz function, taking $\nu = (2-D+d)/2$ in equation (11), we obtain from equation (9) the tadpole part of the

$$m^2(\{L_i\}) = m_0^2 - \frac{\lambda}{(2\pi)^{D/2}}\Bigg[\sum_{n_1=1}^{\infty}\left(\frac{m}{L_1 n_1}\right)^{D/2-1} K_{D/2-1}(mL_1n_1) + \cdots + \sum_{n_d=1}^{\infty}\left(\frac{m}{L_d n_d}\right)^{D/2-1}$$
$$\times K_{D/2-1}(mL_d n_d) + 2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1} K_{D/2-1}\left(m\sqrt{L_i^2n_i^2+L_j^2n_j^2}\right)$$
$$+\cdots+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1} K_{D/2-1}\left(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}\right)\Bigg]$$
$$+\frac{\eta}{2(2\pi)^D}\Bigg[\sum_{n_1=1}^{\infty}\left(\frac{m}{L_1n_1}\right)^{D/2-1} K_{D/2-1}(mL_1n_1)+\cdots+\sum_{n_d=1}^{\infty}\left(\frac{m}{L_dn_d}\right)^{D/2-1} K_{D/2-1}(mL_dn_d)$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1} K_{D/2-1}\left(m\sqrt{L_i^2n_i^2+L_j^2n_j^2}\right)+\cdots+2^{d-1}$$
$$\times\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots L_d^2n_d^2}}\right)^{D/2-1} K_{D/2-1}\left(m\sqrt{L_1^2n_1^2+\cdots L_d^2n_d^2}\right)\Bigg]^2. \quad (16)$$

effective potential in D dimensions with a compactified d-dimensional subspace:

$$U_1(\varphi_0, L_1, ..., L_d) = \frac{\lambda|\varphi_0|^2}{2\,(2\pi)^{D/2}}\Bigg[2^{-D/2-1}m^{D-2}\Gamma\left(\frac{2-D}{2}\right)$$
$$+\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_in_i}\right)^{D/2-1} K_{D/2-1}(mL_in_i)$$
$$+2\sum_{j<i=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2+L_j^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}\left(m\sqrt{L_i^2+L_j^2}\right)+\cdots+2^{d-1}$$
$$\times\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}\left(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}\right)\Bigg], \quad (12)$$

where the K_ν are Bessel functions of the third kind, and we have returned to the original variables, φ_0, λ, and L_i.

We now turn to the 2-loop shoestring diagram contribution to the effective potential, using again the Matsubara-modified Feynman rule prescription for the compactified dimensions. In unbounded space ($L_i = \infty$), it reads

$$U_2(\varphi_0) = \frac{\eta|\varphi_0|^2}{16}\left[\int\frac{d^Dq}{(2\pi)^D}\frac{1}{q^2+m^2}\right]^2, \quad (13)$$

which, after the compactification of d dimensions of linear extensions L_i, $i = 1, \ldots, d$, becomes

$$U_2(\varphi_0, a_1, \ldots, a_d) = \frac{1}{2}g_2|\varphi_0|^2$$
$$\times\mu^{2D-2}a_1\cdots a_d\pi^{D-d}\Bigg[\Gamma\left(\frac{2-D+d}{2}\right)$$
$$\times\sum_{n_1,\ldots,n_d=-\infty}^{\infty}\frac{1}{(a_1n_1^2+\cdots+a_dn_d^2+c^2)^{(2-D+d)/2}}\Bigg]^2, \quad (14)$$

where we have defined φ_0 and a_i as before and the dimensionless quantity $g_2 = (\eta/8\cdot 16\pi^4\mu^{6-2D})$. Equation (8) was also used. The multiple sum above is again the Epstein–Hurwitz zeta function, $Z_d^{c^2}\left(\frac{2-D+d}{2}; a_1\cdots a_d\right)$, given by equation (11) for $\nu = (2-D+d)/2$. In terms of the original variables, φ, η, and L_i, we then have

$$U_2(\varphi_0, L_1, \ldots, L_d) = \frac{\eta|\varphi_0|^2}{4\,(2\pi)^D}\Bigg[2^{-1-D/2}m^{D-2}\Gamma\left(\frac{2-D}{2}\right)$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}\left(m\sqrt{L_i^2n_i^2+L_j^2n_j^2}\right)+\cdots$$
$$+2^{d-1}\times\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\Bigg]^2. \quad (15)$$

Notice that in both equations (12) and (15) there is a term proportional to $\Gamma\left(\frac{2-D}{2}\right)$ which is divergent for even dimensions $D \geq 2$ and should be subtracted in order to obtain finite physical parameters. For odd D, the above gamma function is finite, but we also subtract its term (corresponding to a finite renormalization) for the sake of uniformity. After subtraction we get the renormalized 1- and 2-loop contributions to the effective potential.

Then the physical mass with both renormalized contributions is obtained from equation (4) and also taking into account the contribution at the tree level; it satisfies a generalized Dyson–Schwinger equation depending on the extensions L_i of the confining box:

See equation (16) previous page.

A first-order transition occurs when all the three minima of the potential

$$U(\varphi_0) = \frac{1}{2}m^2(\{L_i\})|\varphi_0|^2 - \frac{\lambda}{4}|\varphi_0|^4 + \frac{\eta}{6}|\varphi_0|^6, \qquad (17)$$

where $m(\{L_i\})$ is the renormalized mass defined above, are simultaneously on the line $U(\varphi_0) = 0$. This gives the condition

$$m^2(\{L_i\}) = \frac{3\lambda^2}{16\eta}. \qquad (18)$$

For $D = 3$, the Bessel functions entering in the above equations have an explicit form, $K_{1/2}(z) = \sqrt{\pi}e^{-z}/\sqrt{2z}$, which is to be replaced in equation (16). Performing the resulting sums, introducing the value of the mass, equation (18), in equation (16), and remembering that $m_0^2 = \alpha(T/T_0 - 1)$, one obtains the critical temperature

$$\begin{aligned} T_c(\{L_i\}) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right)^{-1}\Bigg\{\frac{\lambda}{8\pi\alpha} \\ \times\Bigg[\sum_{i=1}^{d}\frac{1}{L_i}\ln\left(1 - e^{-\sqrt{\frac{3\lambda^2}{16\eta}}L_i}\right) \\ - 2\sum_{j<i=1}^{d}\sum_{n_i,n_j=1}^{\infty}\frac{e^{-m(L_i)\sqrt{L_i^2n_i^2+L_j^2n_j^2}}}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}} \\ - 2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\frac{e^{-\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\Bigg] \\ + \frac{\eta}{64\pi^2\alpha}\Bigg[\sum_{i=1}^{d}\frac{1}{L_i}\ln\left(1 - e^{-\sqrt{\frac{3\lambda^2}{16\eta}}L_i}\right) \\ - 2\sum_{j<i=1}^{d}\sum_{n_i,n_j=1}^{\infty}\frac{e^{-m(L_i)\sqrt{L_i^2n_i^2+L_j^2n_j^2}}}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}} \\ + 2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\frac{e^{-\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\Bigg]^2\Bigg\}\Bigg\}, \end{aligned} \qquad (19)$$

where

$$T_c = T_0\left(1 + \frac{3\lambda^2}{16\eta\alpha}\right) \qquad (20)$$

is the bulk ($L_i \to \infty$) critical temperature for the first-order phase transition.

3 The film, the wire and the grain

Having developed the general case of a d-dimensional compactified subspace, it is now easy to obtain the specific formulas for particular values of d. If we choose $d = 1$, the compactification of just one dimension, let us say, along the x_1-axis, we are considering that the system is confined between two planes, separated by a distance $L_1 = L$. Physically, this corresponds to a film of thickness L and we have that the transition occurs at the critical temperature $T_c^{\text{film}}(L)$ given by

$$\begin{aligned} T_c^{\text{film}}(L) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right)^{-1}\Bigg[\frac{\lambda}{8\pi\alpha L}\ln\left(1 - e^{-\sqrt{\frac{3\lambda^2}{16\eta}}L}\right) \\ + \frac{\eta}{64\pi^2\alpha L^2}\left(\ln(1 - e^{-\sqrt{\frac{3\lambda^2}{16\eta}}L})\right)^2\Bigg]\Bigg\}. \end{aligned} \qquad (21)$$

Let us now take the case $d = 2$, in which the system is confined simultaneously between two parallel planes a distance L_1 apart from one another normal to the x_1-axis and two other parallel planes, normal to the x_2-axis separated by a distance L_2. That is, the material is bounded within an infinite wire of rectangular cross section $L_1 \times L_2$. To simplify matters, we take $L_1 = L_2 = L$ in equation (19) with $d = 2$, and the critical temperature is written in terms of L as

$$\begin{aligned} T_c^{\text{wire}}(L) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right)^{-1} \\ \times\Bigg[\frac{\lambda}{4\pi\alpha L}\Bigg[2\ln\left(1 - e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}}\right) \\ - 2\sum_{n_1,n_2=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{n_1^2+n_2^2}}}{\sqrt{n_1^2+n_2^2}}\Bigg] \\ + \frac{\eta}{32\pi^2\alpha L^2}\Bigg(2\ln\left(1 - e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}}\right) \\ - 2\sum_{n_1,n_2=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{n_1^2+n_2^2}}}{\sqrt{n_1^2+n_2^2}}\Bigg)^2\Bigg]\Bigg\}. \end{aligned} \qquad (22)$$

Finally, we may compactify all three dimensions, which leaves us with a system in the form of a cubic "grain" of some material. The dependence of the critical temperature

on its linear dimension $L_1 = L_2 = L_3 = L$, is given by putting $d = 3$ in equation (19):

$$T_c^{\rm grain}(L) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right)^{-1}\Bigg\{\frac{\lambda}{4\pi\alpha L} \times \Bigg[3\ln\left(1 - e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}}\right) - 2\sum_{j<i=1}^{3}\sum_{n_i,n_j=1}^{\infty}\frac{e^{-\sqrt{\frac{3\lambda^2}{16\eta}}L\sqrt{n_i^2+n_j^2}}}{\sqrt{n_i^2+n_j^2}} - 4\sum_{n_1,\ldots,n_3=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{n_1^2+n_2^2+n_3^2}}}{\sqrt{n_1^2+n_2^2+n_3^2}}\Bigg] + \frac{\eta}{32\pi^2\alpha L^2}\Bigg[3\ln\left(1 - e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}}\right) - 2\sum_{j<i=1}^{3}\sum_{n_i,n_j=1}^{\infty}\frac{e^{-m(L)L\sqrt{n_i^2+n_j^2}}}{\sqrt{n_i^2+n_j^2}} - 4\sum_{n_1,\ldots,n_3=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}}\sqrt{n_1^2+n_2^2+n_3^2}}}{\sqrt{n_1^2+n_2^2+n_3^2}}\Bigg]^2\Bigg\}\Bigg\}. \quad (23)$$

A similar work has been done for a *second-order* transition in either films, wires or grains, obtained by the same methods from the $\lambda\varphi^4$ Ginzburg–Landau model [11]. In this case the $\{L_i\}$ -dependent physical mass has a simpler expression,

$$m_{\rm 2nd}^2(\{L_i\}) = m_0^2 - \frac{\lambda}{(2\pi)^{D/2}}\Bigg[\sum_{n_1=1}^{\infty}\left(\frac{m}{L_1 n_1}\right)^{D/2-1} \times K_{D/2-1}(mL_1n_1) + \cdots + \sum_{n_d=1}^{\infty}\left(\frac{m}{L_d n_d}\right)^{D/2-1} K_{D/2-1}(mL_d n_d) + 2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1} \times K_{D/2-1}\left(m\sqrt{L_i^2n_i^2+L_j^2n_j^2}\right) + \cdots + 2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1} \times K_{D/2-1}\left(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}\right)\Bigg], \quad (24)$$

from which, taking all L_i's equal to L and going to the limit $m_{\rm 2nd}^2(\{L_i\}) \to 0$, formulas for the transition temperature for films, wires and grains can be obtained. All of them have the same functional dependence on the linear dimension L. In all cases studied there, it is found that the boundary-dependent critical temperature decreases linearly with the inverse of the linear dimension L,

$$T_c^{\rm 2nd}(L) = T_0 - \frac{C_d\lambda}{\alpha L}, \quad (25)$$

where α and λ are the Ginzburg–Landau parameters, T_0 is the bulk transition temperature and C_d is a constant equal to 1.1024, 1.6571 and 2.6757 for $d = 1$ (film), $d = 2$ (square section wire) and $d = 3$ (cubic grain), respectively.

Comparing equations (21)–(23) with equation (25), we see that in all the cases (a film, a wire or a grain), there is a sharp contrast between the simple inverse linear behavior of $T_c(L)$ for second-order transitions and the rather involved dependence on L of the critical temperature for first-order transitions. These two types of behavior prompt us to try to clarify the subject further, by comparing the theoretical curves with experimental data for superconducting materials. However, as far as we know, no available data exist for superconducting grains. We shall thus consider the situations of bounded systems in the form of a film or of a wire. In so doing, we can explicitly compare the forms of the $T_c(L)$ curves for both first- and second-order transitions, and also exhibit the degree of agreement between our theoretical expressions for the first-order critical temperature and some experimental results obtained from superconducting films and wires.

To start, we mention the generalization of Gorkov's [17–19] microscopic derivation for the $\lambda\varphi^4$ model in order to include the additional interaction term $\eta\varphi^6$ in the free energy [13]. The interest here is to determine the phenomenological constant η as a function of the microscopic parameters of the material, in an analogous way as has been done for the constant λ in the $\lambda\varphi^4$ model. This leads to [13],

$$\alpha = 1 \quad \lambda \approx 111.08\left(\frac{T_0}{T_F}\right)^2, \qquad \eta \approx 8390\left(\frac{T_0}{T_F}\right)^4, \quad m_0^2 = \frac{T}{T_0} - 1, \quad (26)$$

where T_F is the Fermi temperature and T_0 is the temperature parameter introduced in equation (1), which can be obtained from the first-order bulk critical temperature by means of equation (20).

By replacing the above constants in equation (21), we get the critical temperature as a function of the film thickness and in terms of tabulated microscopic parameters for specific materials.

We remark that Gorkov's original derivation of the phenomenological constants is valid only for perfect crystals, where the electron mean free path l is infinite. However, we know that in many superconductors the attractive interaction between electrons (necessary for pairing) is brought about indirectly by the interaction between the electrons and the vibrating crystal lattice (phonons). The presence of impurities within the crystal lattice modifies the interaction between electrons and phonons, with the consequence of making the electron mean free path finite. In fact the dieter is the sample, shorter the mean free path

becomes [19]. The Ginzburg–Landau phenomenological constants λ and η and the coherence length are somehow related to the interaction of the electron pairs with the crystal lattice and the impurities. A way of taking these facts into account preserving the form of the Ginzburg–Landau free energy is to modify the intrinsic coherence length ξ_0 and the coupling constants. Accordingly [19], $\xi_0 \to \rho^{1/2}\xi_0$, $\lambda \to 2\rho^{-3/2}\lambda$ and $\eta \to 4\rho^{-3}\eta$, where $\rho \approx 0.18R^{-1}$, with $R = \xi_0/l$, where $\xi_0 = 0.13(\hbar v_F/k_B T_0)$. Then, it can be shown that equation (21) becomes [13],

$$T_c^{\rm film}(L) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta}\right)^{-1}\Bigg[\frac{2R\lambda}{0.18\cdot 8\pi}\frac{\xi_0}{L} \times \ln\left(1 - e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right) + \frac{4R^2\eta}{0.18^2\cdot 32\pi^2}\left(\frac{\xi_0}{L}\right)^2 \times \left(\ln\left(1 - e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right)\right)^2\Bigg]\Bigg\}. \quad (27)$$

Also for realistic samples other effects, such that of the substrate over which the superconductor film is deposited, should be taken into account. In the context of our model, however, we are not able to describe such effects at a microscopic level. We therefore assume that they will be translated in changes on the values of the coupling constants λ and η. So, we propose as an *Ansatz* the rescaling of the constants in the form $\lambda \to a\lambda$ and $\eta \to a^2\eta$. We may still combine both parameters R and a as $r = aR$. equation (27) is then written as

$$T_c^{\rm film}(L) = T_c\Bigg\{1 - \left(1 + \frac{3\lambda^2}{16\eta}\right)^{-1}\Bigg[\frac{2r\lambda}{0.18\cdot 8\pi}\frac{\xi_0}{L} \times \ln\left(1 - e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right) + \frac{4r^2\eta}{0.18^2\cdot 32\pi^2}\left(\frac{\xi_0}{L}\right)^2 \times \left(\ln\left(1 - e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right)\right)^2\Bigg]\Bigg\}. \quad (28)$$

In Figure 1 we plot equation (28) to show the behavior of the transition temperature as a function of the thickness for a film made from aluminum. The values for Al of the Fermi temperature, the bulk critical temperature and Fermi velocity are $T_F = 13.53 \times 10^4$ K, $T_c = 1.2$ K, and $v_F = 2.02 \times 10^6$m/s, respectively.

We see from the figure that the critical temperature grows from zero at a nonnull minimal allowed film thickness above the bulk transition temperature T_c as the thickness is enlarged, reaching a maximum and afterwards starting to decrease, going asymptotically to T_c as $L \to \infty$.

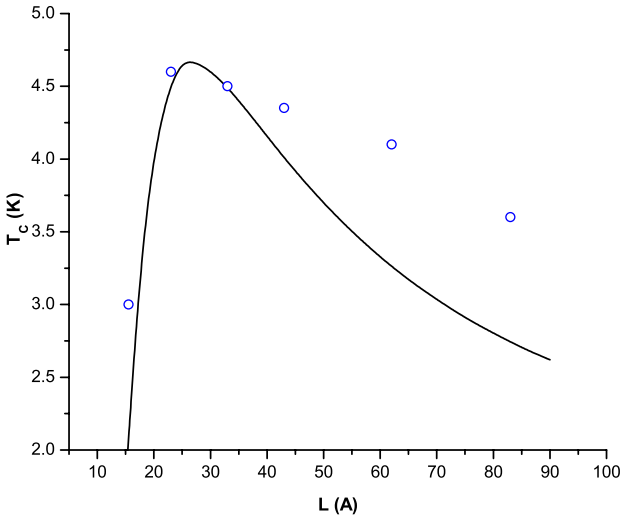

Fig. 1. Critical temperature $T_c^{\rm film}$(K) as function of thickness L (Å), from equation (28) and data from reference [20] for a superconducting film made from aluminum.

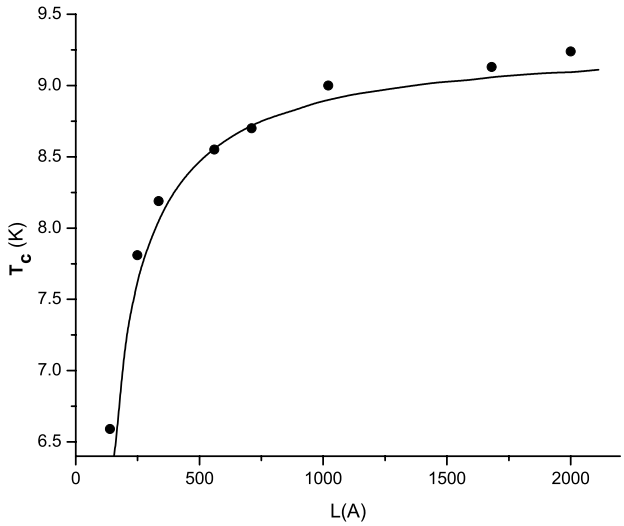

Fig. 2. Critical temperature T_c (K) as a function of the thickness L (Å) for a second-order transition, as theoretically predicted in reference [9]. Dots are experimental data taken from reference [21] for a superconducting film made from niobium.

We also plot for comparison some experimental data obtained from reference [20]. We see that our theoretical curve is in qualitatively good agreement with measurements, especially for thin films.

This behavior may be contrasted with the one shown by the critical temperature for a *second-order* transition. In this case, the critical temperature increases monotonically from zero, again corresponding to a finite minimal film thickness, going asymptotically to the bulk transition temperature as $L \to \infty$. This is illustrated in Figure 2, adapted from reference [9], with experimental data from [21]. (Such behavior has also been experimentally found by some other groups for a variety of transition-metal materials, see Refs. [25–27].) Since in the present

work a first-order transition is explicitly assumed, it is tempting to infer that the transition described in the experiments of reference [20] is first order. In other words, one could say that an experimentally observed behavior of the critical temperature as a function of the film thickness may serve as a possible criterion to decide about the order of the superconductivity transition: a monotonically increasing critical temperature as L grows would indicate that the system undergoes a second-order transition, whereas if the critical temperature presents a maximum for a value of L larger than the minimal allowed one, this would be signaling the occurrence of a first-order transition.

Let us now consider a sample of superconducting material in the form of an infinitely long wire with a cross section of side L. The same arguments and rescaling procedures used precedingly for films apply equally in the present situation. In this way, equation (22) is accordingly modified. It assumes the form

$$T_c^{\rm wire}(L) = T_c\Bigg\{1 - \left(1+\frac{3\lambda^2}{16\eta}\right)^{-1}\Bigg[\frac{2r\lambda}{0.18\cdot 8\pi}\frac{\xi_0}{L} \times \Bigg[2\ln\left(1-e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right) - 2\sum_{n_1,n_2=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}\sqrt{n_1^2+n_2^2}}}{L\sqrt{n_1^2+n_2^2}}\Bigg] + \frac{4r^2\eta}{0.18^2\cdot 32\pi^2}\left(\frac{\xi_0}{L}\right)^2\Bigg[2\ln\left(1-e^{-\frac{L}{\xi_0}\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}}\right) - 2\sum_{n_1,n_2=1}^{\infty}\frac{e^{-L\sqrt{\frac{3\lambda^2}{16\eta}\frac{R}{0.18}}\sqrt{n_1^2+n_2^2}}}{L\sqrt{n_1^2+n_2^2}}\Bigg]^2\Bigg]\Bigg\}. \quad (29)$$

Notice that, due to the presence of the exponentials, the double series in equation (29) is convergent. Therefore, they can be truncated at some finite value for n_1 and n_2, so that a plot of the curve $T_c^{\rm wire}(L)$ vs. L can be drawn. In fact, the series are rapidly convergent and no detectable difference exists if we take the sums over n_1 and n_2 up to 50 or a higher number. In Figure 3 this curve is plotted and compared with experimental data from references [22,23] for an aluminum wire. Here, we have used the same tabulated values for T_F, T_c and v_F for aluminum as in the case of films. Also, for the parameter R a larger value than the corresponding one for films ($R_{\rm wire} = 20\,R_{\rm film}$) is taken. This is to account for the fact that samples in the form of wires are more sensitive to the presence of impurities than in the case of films [24]. From Figure 3, we then notice that, for not extremely thin wires, the data agrees quite well with the theoretical curve. We see that the theoretical predicted behavior of the critical temperature as a function of the square root of the cross section area (for us, the transverse linear dimension L) is qualitatively of the same type we found for films. Therefore, if one follows the same line of reasoning we have done for films, one may conclude that the phase transition for these superconducting

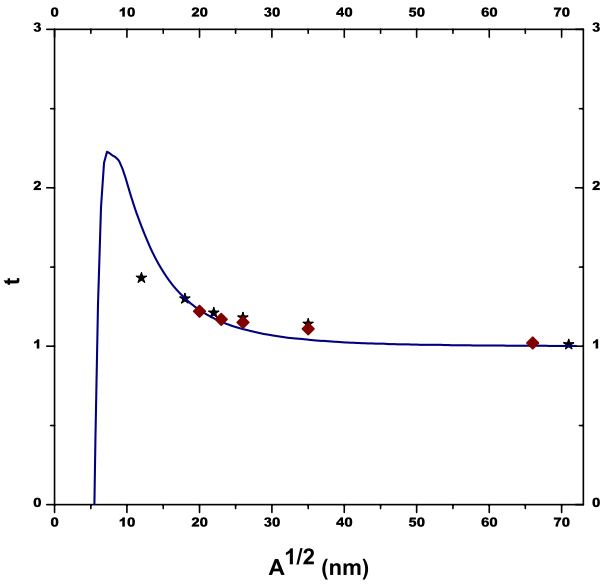

Fig. 3. Reduced critical temperature $t = T_c^{\rm wire}/T_{\rm bulk}$ as a function of the square root of the cross section $A^{1/2}$ (nm), from equation (29) for an Al wire (the solid curve). The diamond symbols are data from reference [22] and the star symbols are data from reference [23]. We have used $r = 150\times 10^4$ and $R \approx 23$.

aluminum wires is first order, just as for aluminum films. This conjecture is reinforced, if one remembers that equation (25) for second-order transitions is equally applicable to wires, showing a similar behavior as that illustrated in Figure 2, in which the curve approaches the bulk critical temperature from below. However, it is clear from the data that the critical temperature takes higher values as L is decreased, thus being incompatible with the expected behaviour of a second order transition.

4 Concluding remarks

Studies on the dependence of the critical temperature for films with its thickness have been done in other contexts and approaches, different from the one we adopt. For instance in references [1,7] an analysis of the renormalization group in finite-size geometries can be found. Also, such a dependence has been investigated in [32,33,25,26] from both experimental and theoretical points of view, explaining this effect in terms of proximity, localization and Coulomb interaction. In particular, reference [32] predicts, as our model also do, a suppression of the superconducting transition for thicknesses below a minimal value. More recently in reference [22] the thickness dependence of the critical temperature is explained in terms of a shape-dependent superconducting resonance, but no suppression of the transition is predicted or exhibited.

In this paper we have adopted a phenomenological approach, discussing the $\left(\lambda|\varphi|^4+\eta|\varphi|^6\right)_D$ theory compactified in $d \le D$ Euclidean dimensions. We have presented a general formalism which, in the framework of the

Ginzburg–Landau model, is able to describe phase transitions for systems defined in spaces of arbitrary dimension, some of them being compactified. We have focused on the situations with $D = 3$ and $d = 1, 2, 3$, corresponding (in the context of condensed-matter systems) to films, wires and grains, respectively, undergoing phase transitions which are supposed to be described by (mean-field) Ginzburg–Landau models. We have parameterized the bare mass term in the form $m_0^2 = \alpha(T/T_0 - 1)$, with $\alpha > 0$ and T_0 being a parameter with the dimension of temperature, thus placing the analysis within the Ginzburg–Landau framework. This generalizes previous works dealing with first- and second-order transitions and low-dimensional compactified subspaces [13,8, 11] . Such a generalization is far from being trivial, since it involves extensions to several dimensions of the one-dimensional mode-sum regularization described in reference [16]. These extensions require, in particular, the definition of symmetrized multidimensional Epstein–Hurwitz functions with no analog in the one-dimensional case. It is this kind of mathematical framework that allows us to obtain the general formula (19), which may be particularized to films, wires and grains, thereby implying the peculiar forms of the critical temperature as a function of the linear dimension L, for the three physically interesting cases.

It should be observed the very different form of equations (21)–(23) when compared with the corresponding ones for second-order transitions given by equation (25), obtained within the Ginzburg–Landau φ^4 theory. In all cases, the functional form of the dependence of the critical temperature $T_c(L)$ on the linear dimension L is of the following type: it grows from zero at a nonnull minimal allowed value of L below the bulk transition temperature T_c as L is enlarged, reaching a maximum above T_c and afterwards starting to decrease, going asymptotically to T_c as $L \to \infty$. Equation (21) is in qualitatively good agreement with measurements [20] taken for a superconducting aluminum film, especially for thin ones. Moreover, experimental data published in very recent years for an Al superconducting wire [22,23] show good accordance with equation (22). Due to the extreme difficulties in preparing very thin wires, however, there is an unfortunate lack of data for $L \lesssim 15$ nm, which prevents the testing of the characteristic behavior of T_c we expect in this range of values, with a sudden drop to zero of T_c after it reaches a maximum value above the bulk one. This is a very contrasting behavior with that of the critical temperature for materials displaying a second-order phase transition [9], for which the critical temperature increases monotonically from zero, again corresponding to a finite minimal film thickness, going to the bulk transition temperature as $L \to \infty$. Such behavior may indicate that from the form of the dependence of the critical temperature on the size of the system, the order of the transition the system undergoes could be inferred. Finally we should mention the important point that *hysteresis* is a characteristic feature of a first-order transition. In our case, it would mean that the transition temperature in the direction from the normal phase to the superconducting phase (let's call it T_c^{NS}) is different from the critical temperature in the inverse way (T_c^{SN}). To our knowledge, the experiments investigating the thickness-dependent transition temperature are only from the normal state to the superconducting one, so they do not show hysteresis. We have not found, at least in the papers that are useful for us, experimental studies on the comparison of the critical temperatures T_c^{NS} and T_c^{SN}. For us, remembering equations (19) and (20), such a study would require separate calculations of the the Ginzburg-Landau phenomenological parameters λ, α and η for the transition in the directions NS and SN.

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