Analysis of the perturbation series for the specific heat of a thin-film superconductor near H_{c2}

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The asymptotic perturbation series developed over many years from the Landau-Ginzburg theory is used to study the specific heat of a thin-film superconductor in a magnetic field. It is found that rewriting the series as an expansion in the entropy improves the self-consistency of its Padé or Padé-Borel resummations at low temperatures. However, there is a discrepancy between Monte Carlo data and the series resummations, possibly due to saddle-point contributions that are only a finite energy away from the point about which the perturbation expansion is performed. Our expansion is also used on the exactly soluble zero-dimensional Landau-Ginzburg model, our toy model. The results of the Padé and Padé-Borel resummations are more accurate than previous methods, but still do not converge to the exact low-temperature limit. The δ expansion and Stevenson transformation are tried on the toy model but the former is discarded because its convergence is too slow to be practical and the latter because results are very poor in the temperature region where the Borel sum fails to converge to the exact result. We conclude that no satisfactory resummation procedure exists for this problem. Finally Monte Carlo data are compared with recent experimental results and the agreement is found to be poor at low temperatures. The extension of our analysis to the series for bulk systems has been made. No strong evidence for a transition could be found.

I. INTRODUCTION

The question of whether a thin-film type-II superconductor in a magnetic field has a phase transition is controversial. The popular belief is that below a nonzero temperature (T_m) the vortices form a triangular (Abrikosov) lattice. The melting of this lattice has been studied theoretically by Huberman and Doniach[1] and Fisher,[2] who proposed dislocation unbinding as a melting mechanism. Various Monte Carlo simulations on approximations to the full Landau-Ginzburg partition function and experimental studies claim evidence for the existence of the Abrikosov lattice phase. However, it has been argued by one of us[3] that below four dimensions thermal fluctuations destroy the superconductor phase coherence. (This falls to three dimensions if the vector potential $\mathbf{A}$ is fixed.) It seems natural that the absence of long-range phase coherence in two dimensions should be accompanied by the destruction of the vortex lattice for a thin film. This view is supported by a recent Monte Carlo simulation[4] in which no evidence for a phase transition was found, although as the temperature was lowered it was observed that latticelike order existed over longer length scales.

Ruggeri and Thouless[5] and more recently Hikami and co-workers[6–8] developed a perturbation series for the free energy starting from Landau-Ginzburg theory. The series is asymptotic so that in order to study the low-temperature region where a transition might be expected, extrapolation techniques such as Padé or Padé-Borel approximants must be employed. The question as to which resummation procedure of the series works best and whether it converges to the correct result is the chief topic of this paper.

We shall begin by considering a variable transformation which allows us to rewrite the series in terms of the entropy, which for this special case is the renormalized propagator. This means that we have included all possible loop insertions—as compared with just the one-loop insertions of the original series of Refs. 5–8. As a consequence we have an expansion that is effectively in terms of the skeleton Feynman diagrams.

The modified series is found to have improved self-consistency when extrapolated by Padé or Padé-Borel methods to the low-temperature region. However, although the agreement with the Monte Carlo data is good, there is a noticeable discrepancy at low temperatures if we do not impose the limiting low-temperature behavior by hand. Consequently our work can provide no evidence for or against a phase transition in thin films.

In three dimensions we cannot consider the variable transformation to be equivalent to a skeleton-graph expansion, but this does not prevent us from carrying out the transformation. Analysis of the series does not provide very strong evidence for a phase transition in three dimensions, in contrast with the conclusions of Ref. 7.

The zero-dimensional Landau-Ginzburg theory[9] for this problem is exactly soluble and thus became our toy model. It is found that the skeleton-graph expansion performs significantly better than the original series, but high-order Padé approximants have a low-temperature limit 10% greater than the exact answer. Analysis of the toy model suggests that the problems stem from a contribution of the stationary point of the action which switches in at the mean-field transition temperature. It can be shown that saddle points of the finite action (or energy) will always make a contribution to the partition function, and hence the free energy. The finite-energy stationary points, which we shall show also exist in two dimensions (but not three), are the source of the discrepancy between the Padé and Padé-Borel resummations of the skeleton-graph expansion and the exact result in the toy model. *If this is also true for two dimensions, it implies that the resummed perturbation series will not converge to the correct low-temperature limit in two dimensions no matter how many terms are supplied, unless a better technique of resummation can be found.* Note that just because a series is Borel summable (as is the case of all the series considered here[8]), this does not imply that the Borel sum is an exact result.

In a search for better methods of analysis, two have been tested on the toy model, but have not been transferred to the two-dimensional case because of their poor performances. These were the δ expansion,[10] which has been proven to converge to the exact result in a similar toy but does so too slowly to be of any use in the two-dimensional case, and the Stevenson transformation,[11] which did not produce sensible results below the mean-field transition temperature. We are unaware of any other extrapolation techniques which might yield better results, for series of the length available to us.

The Monte Carlo results are also compared with recent experimental results,[12] for a superconductor-insulator multilayer, where the layers are considered to have two-dimensional (2D) character. The agreement is very poor. Possible sources of the discrepancy are the lack of disorder in the theoretical model (which is still being investigated) or the three-dimensional character of the stack of layers.

II. PREVIOUS WORK

We start from the Landau-Ginzburg free-energy functional

$$\frac{F[\psi(r)]}{k_B T_c} = \int d^3r \left(\alpha(T)\,|\psi|^2 + \beta\,\frac{|\psi|^4}{2} + \frac{|(-i\hbar\nabla - 2e\mathbf{A})\psi|^2}{2\mu} \right), \tag{2.1}$$

where $\alpha(T)$, β, μ are our phenomenological parameters. The temperature dependence of $\alpha(T)$ is taken to be linear, $\alpha(T) = \alpha'(T - T_c)$. For a sufficiently thin film fluctuations in the vector potential $\mathbf{A}$ can be ignored. This is justified because the range of variation of fluctuations in $\mathbf{A}$ is of order λ^2/L_z where L_z is the film thickness and λ is the bulk penetration depth. This range is usually of macroscopic size. The free energy is then defined by the functional integral

$$\frac{G_{2\text{D}}}{kT_c} = -\ln \int \mathcal{D}\psi\,\mathcal{D}\psi^* \exp\left(-\frac{F[\psi(r)]}{k_B T_c}\right). \tag{2.2}$$

For convenience we will work in the symmetric gauge $\mathbf{A} = B(-y, x, 0)/2$ where B is the uniform field, applied perpendicular to the film. We are now able to rewrite the free energy in terms of the reduced temperature,

$$\alpha_h = \alpha + eB\hbar/\mu\,, \tag{2.3}$$

which is zero along the H_{c_2} line. To further simplify the calculation the order parameter ψ will be taken to be in the lowest Landau level, so that

$$\left(-i\hbar\frac{\partial}{\partial x} + \hbar\frac{\partial}{\partial y} - eiBx + eBy\right)\psi = 0\,. \tag{2.4}$$

This approximation is valid providing[13]

$$B^2 \gg \frac{8\pi k T_c \kappa^2 \alpha_h^2}{\beta} \tag{2.5}$$

(κ is the Ginzburg ratio), which is a regime explored in recent experimental work.[12] For a sufficiently thin film variations of ψ and ψ^* along the magnetic field direction can be neglected. In Ref. 5 the free energy (now per unit volume) was expressed as

$$\frac{G_{2\text{D}}}{kT_c} = \frac{eB}{L_z\pi\hbar}\left[-\frac{1}{2}\ln\left(\frac{2\pi^3 L_z\hbar x}{\beta e B}\right) + f_{2\text{D}}(x)\right], \tag{2.6}$$

where x is defined by the relationship

$$\alpha_h = \sqrt{\frac{\beta e B}{\pi L_z \hbar}}\,\frac{(1-4x)}{\sqrt{2x}} \tag{2.7}$$

and the function $f_{2\text{D}}(x)$ is not known exactly but a perturbation series for it can be obtained in terms of β through the use of Feynman diagrams.

Ruggeri and Thouless[5] calculated the perturbation series up to 6th order and this was subsequently extended to 11th order by Brèzin, Fujita, and Hikami,[8] viz.,

$$\begin{aligned} f_{2\text{D}}(x) = &-2x - x^2 + \tfrac{38}{9}x^3 - \tfrac{1199}{30}x^4 + 471.396594517x^5 \\ &-6471.56257496x^6 + 101279.327846x^7 \\ &-1779798.78759x^8 + 34709019.6144x^9 \\ &-744093435.668x^{10} + 17399454123.5x^{11} \\ &+O(x^{12}). \end{aligned} \tag{2.8}$$

Throughout this paper we will work with dimensionless variables and thermodynamic functions, such that up to a constant in the free energy we have

$$g_{2\text{D}} = \frac{L_z\pi\hbar}{eB}G_{2\text{D}} = -\frac{1}{2}\ln(x) + f_{2\text{D}}(x),$$
$$\alpha_T = \sqrt{\frac{\pi L_z\hbar}{\beta e B}}\,\alpha_h = \frac{1-4x}{\sqrt{2x}}\,, \tag{2.9}$$

with the entropy defined by

$$s = -\frac{dg_{2\text{D}}}{d\alpha_T}. \tag{2.10}$$

The chief thermodynamic function that we consider is the specific heat, normalized by its mean-field discontinuity, viz.,

$$\Delta C = \frac{kT_c^2(\alpha')^2}{\beta\beta_a} . \tag{2.11}$$

β_a is the minimum value of the Abrikosov factor,

$$\int |\psi|^4 d^3r / \left(\int |\psi|^2 d^3r\right)^2 . \tag{2.12}$$

This minimum is found to correspond to a regular triangular lattice of the zeros of ψ, i.e., for the vortices, when $\beta_a \approx 1.1596$. This means that the normalized specific heat in our units is

$$\frac{C}{\Delta C} = -\beta_a \frac{d^2 g_{2D}}{d\alpha_T^2} . \tag{2.13}$$

In three dimensions the dimensionless free energy g_{3D} and temperature α_T are defined by

$$g_{3D} = \left(\frac{eBk_BT\sqrt{m}}{\pi\hbar^2}\right)^{4/3}, \quad G_{3D} = \frac{1+f_{3D}(x)}{(2x)^{1/3}} ,$$
$$\alpha_T = \left(\frac{4\pi\hbar^2}{\beta_k eBk_BT\sqrt{2m}}\right)^{2/3}, \quad \alpha_h = \frac{1-8x}{(2x)^{2/3}} , \tag{2.14}$$

where G_{3D} is the free energy of Ruggeri and Thouless,[5] apart from an additive constant, and α_h is their temperature variable. The perturbation series was originally calculated by Ruggeri and Thouless up to sixth order[5] and later extended to ninth order by Hikami and Fujita:[6]

$$\begin{aligned} f_{3D} = &-2x - \tfrac{1}{2}x^2 + \tfrac{19}{12}x^3 - \tfrac{18241}{1440}x^4 + 125.59552619x^5 \\ &-1430.5928959x^6 + 18342.7659972x^7 \\ &-261118.67703x^8 + 4084812.3074x^9. \end{aligned} \tag{2.15}$$

Equation (2.8) is an asymptotic divergent series and resummation techniques must be employed in order to study the behavior of thermodynamic properties. In previous work these have been of the Padé and Padé-Borel type with usually the additional constraint that at low temperatures the mean-field result should be recovered.[5,6,8,14] This condition becomes the requirement that the normalized specific heat should tend to unity in the low-temperature region when $\alpha_T \to -\infty$.

Ruggeri and Thouless imposed the low-temperature constraint by subtracting the mean-field limit $(-4x/\beta_a)$ from the free-energy series. This series is required to have a low-temperature limit of zero, which was enforced by choosing an $[N-1, N]$ Padé approximant which automatically goes to zero for large x. The full result for the free energy $f_{2D}(x)$ was then found by reintroducing the mean-field limit.

In an alternative approach, Hikami and Fujita[6] constrained their Padé approximants by assuming the form

$$f_{2D}(x) = -2\int_0^\infty dx\, e^{-t/x} \frac{\sum_0^N a_m x^m}{(1+\sum_1^N b_m x^m)}, \tag{2.16}$$

with the requirement that $a_N = (2/\beta_a)b_N$. (The coefficients of the Padé approximants will always be labeled such that a_m is the coefficient of x^m and the order in this example would be described as $[N, N]$.)

We have found that the manner in which the mean-field constraint is imposed has an effect on the specific-heat function even close to $\alpha_T = 0$—the mean-field transition temperature. However, for any particular method, imposing the constraint does improve the mutual consistency of the approximants. The mean-field result was not reproduced exactly by the unconstrained approximants, although these do come closer with increasing order N.

It is evident that a more reliable approach could be obtained by imposing more information about the low-temperature behavior, and to this end, Ruggeri[15] studied fluctuations around the flux lattice. He obtained the one-loop correction (Gaussian fluctuation) to the mean-field expression for the entropy so that, in our units, the entropy s has a low-temperature behavior of the form

$$s = \frac{\alpha_T}{\beta_a} - \frac{1}{\alpha_T} \quad \text{as } \alpha_T \to -\infty . \tag{2.17}$$

This allowed him to further constrain the Padé approximants.[14] He suggested the correction introduced by this procedure as an explanation for the peak in the specific-heat curve.

More recently Hikami, Fujita, and Larkin[7] have also studied the low-temperature behavior, but they used an earlier expression of Thouless[16] such that their entropy expression is

$$s = \frac{\alpha_T}{\beta_a} + \frac{\sqrt{x}}{\beta_a(1+4x)} \to \frac{\alpha_T}{\beta_a} - \frac{1}{\sqrt{2}\beta_a\,\alpha_T} \quad \text{as } x\to\infty,\ \alpha_T \to -\infty . \tag{2.18}$$

The two expressions for s are inequivalent. We suspect Eq. (2.17) is correct, though we make no use of either equation in our work.

A. Toy model

It was noted by Bray[9] that one can obtain a series for the zero-dimensional Landau-Ginzburg system which is of the same form as that for the thin-film superconductor. This theory has the advantage of being exactly soluble and so has been used as a toy model to test the validity of various resummation schemes. Since none of the standard methods give convincing results for the toy model, this casts considerable doubt on their validity for the two-dimensional case.

In the toy model one starts with the free energy defined by

$$g_{0D}(x) = -\tfrac{1}{2}\ln(x) + f_{0D}(x), \tag{2.19}$$

where f_{0D} is given by

$$f_{0D} = -\ln\left[\int_0^\infty dt\, \exp\left[-(1-4x)t - xt^2\right]\right] . \tag{2.20}$$

This has been derived from the expression for the zero-dimensional partition function,

$$Z = \int\int d\psi\, d\psi^* e^{-\psi\psi^* - g\psi^2\psi^{*2}}. \tag{2.21}$$

The analog of the free-energy series f_{2D}, [Eq. (2.8)] is

$$\begin{aligned} f_{0D}(x) = & -2x - 2x^2 + \tfrac{40}{3}x^3 - 196x^4 + \tfrac{18208}{5}x^5 \\ & -\tfrac{245408}{3}x^6 + \tfrac{15111808}{7}x^7 - 65488928x^8 \\ & +\tfrac{20211520000}{9}x^9 - \tfrac{429568420352}{5}x^{10} \\ & +\tfrac{39907677104128}{11}x^{11} + O(x^{12}), \end{aligned} \tag{2.22}$$

and the variable corresponding to α_T, i.e., the effective temperature, is $y = (1-4x)/\sqrt{2x}$. The exact solution for g_{0D} is most readily expressed in terms of y and is

$$g_{0D}(y) = -\ln[e^{y^2/2}\,\mathrm{erfc}(y/\sqrt{2})] = -\ln[w(iy/\sqrt{2})], \tag{2.23}$$

where $w(z)$ is as defined in Ref. 18 [Eq. (7.1.3)]. The analogs of the entropy and normalized specific heat in zero dimensions are defined by

$$s = -\frac{dg_{0D}}{dy} \qquad \frac{C}{\Delta C} = -\frac{d^2 g_{0D}}{dy^2}. \tag{2.24}$$

III. THE SKELETON-GRAPH METHOD

The weaknesses in the standard resummation procedures used in Refs. 5, 6, and 8 suggested that a more robust method is required. To this end the series of Eq. (2.8) was rewritten as one for the reduced temperature α_T in terms of the entropy,

$$\alpha_T = \sum_{n=0}^{12} a_n s^{(2n-1)}. \tag{3.1}$$

This was then rearranged for the entropy in terms of the renormalized propagator (the entropy) for all but the initial propagator,

$$s = \frac{1}{\alpha_T}\sum_{n=0}^{12} a_n s^{2n}. \tag{3.2}$$

In terms of diagrams this corresponds to Fig. 1, where the thick line indicates the renormalized propagator (s) and the thin line the bare propagator ($1/\alpha_T$). The skeleton method effectively allows us to work to a higher order in the coupling constant than in the Hartree-Fock resummation used in Refs. 5 and 6. This first becomes apparent with the three-vertex diagrams. In the Hartree-Fock scheme terms of the form in Fig. 2(a) are included but the term in Fig. 2(b) must be calculated separately. In the skeleton expansion this diagram is already included. (The reduction in the number of diagrams becomes significant at higher orders, so the scheme could be of further use if more terms in the series were needed.) This diagrammatic interpretation of the series inversion is only possible because the renormalized propagator is directly proportional to the bare propagator.[17]

The algebraic techniques required to invert the series are straightforward, but because the original polynomial is 11th order, the evaluation of the new series was

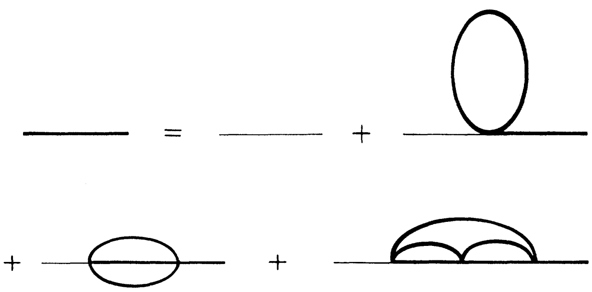

FIG. 1. The skeleton-graph expansion in terms of loop diagrams up to three vertices.

done using MATHEMATICA. From the original Landau-Ginzburg equation (2.1) it can be shown that the entropy can be written as a series in odd powers of $1/\alpha_T$,

$$s = \sum_{n=1}^{12} b_n \left(\frac{1}{\alpha_T}\right)^{(2n-1)}, \tag{3.3}$$

where α_T is defined in Eq. (2.9).

It is also possible, however, to write the entropy as a

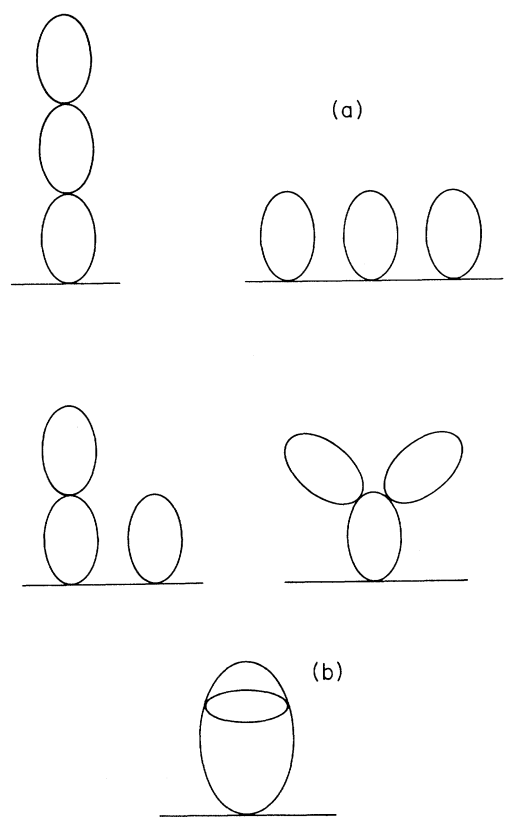

FIG. 2. (a) Graphs which are included in both the Hartree-Fock and skeleton expansions. (b) An example of a three-vertex graph which is included in the skeleton-graph expansion but must be calculated separately in the Hartree-Fock expansion.

polynomial in x with known coefficients using the free-energy perturbation series

$$s = \sqrt{2x}(2xf'_{2D} - 1)/(1+4x) . \quad (3.4)$$

By equating the expressions of Eqs. (3.3) and (3.4), we can determine the coefficients b_n. Having done this, the series in terms of α_T [Eq. (3.3)] can be written in terms of s by inversion, leading to

$$\alpha_T = -\frac{1}{s}\,[1 - 2s^2 + s^4 - \tfrac{19}{6}s^6 + 15.9833333333333s^8 - 105.6447691199s^{10} + 839.4513161383306s^{12} - 7668.3830488111s^{14} + 78436.36669669s^{16} - 883237.5856207423s^{18} + 10822981.33681286s^{20} - 143118270.587s^{22} + O(s^{24})] . \quad (3.5)$$

The same procedure has been carried out for the toy model, using Eq. (2.20), to obtain an equation for the entropy analogous to that of Eq. (3.4). The resulting series to the same order as the two-dimensional series is

$$y = -\frac{1}{s}\,[1 - 2s^2 + 2s^4 - 10s^6 + 82s^8 - 898s^{10} + 12018s^{12} - 187626s^{14} + 3323682s^{16} - 65607682s^{18} + 1424967394s^{20} - 33736908874s^{22} + O(s^{24})] . \quad (3.6)$$

Higher-order terms are readily obtainable and we have in fact calculated the series up to s^{44}.

In the three-dimensional case of a bulk superconductor, it is possible to carry out a series inversion analogous to that performed in two dimensions. However, in three dimensions we cannot consider it as a skeleton-graph expansion because there is an additional wave-vector integral over k_z, the wave vector associated with changes in the order parameter ψ with height, and thus, for example, the entropy at lowest order is related to α_T by

$$s \sim \int \frac{dk_z}{2\pi}\frac{1}{(k_z^2 + \alpha_T)} , \quad (3.7)$$

which prevents there being a simple relationship between the renormalized propagator and the entropy. Examination of the integral shows that in three dimensions $s \sim 1/\sqrt{\alpha_T}$, suggesting that s^2 will be the appropriate variable for the series inversion—this is indeed found to be the only simple variable with which it is possible to perform the inversion. The resulting series is

$$\alpha_T = \frac{1}{4s^2}\,[1 + 32s^3 + 80s^6 + \tfrac{4864}{3}s^9 + 53742.577772s^{12} + 2334728.2603s^{15} + 121469761.94s^{18} + 7228438383.6s^{21} + 479024071485s^{24} + O(s^{27})] \quad (3.8)$$

where s is always negative, and so the series is in fact of the alternating type and is Borel resummable.[8]

IV. ANALYSIS OF THE SKELETON-GRAPH SERIES AND COMPARISON WITH PREVIOUS METHODS

A. Two-dimensional case

Published results for the specific heat of the thin-film superconductor have used the toy model as their benchmark.[5,14] We shall also compare our results with the Monte Carlo values obtained in Ref. 4. The Monte Carlo simulation lends itself most readily to a determination of the entropy. The specific-heat function can be obtained by differentiation of the entropy but because of a scarcity of points a smooth curve could only be obtained by first fitting a cubic spline. Hence the comparisons with the Monte Carlo itself are made in terms of the entropy which is the raw data. However, in order to facilitate comparison with other papers, the remaining results are presented in terms of the specific heat with the proviso that the Monte Carlo curve is only a guideline, due to the inadequacies of the cubic spline.

Apart from the overall external factor of $-1/s$, the terms in the skeleton series seem to have a dominant high-n behavior $a_n \sim (-1)^n n!$, with a_n defined by Eq. (3.1). This indicates that rewriting the reduced temperature α_T in terms of a Padé-Borel form using s^2 as the variable would be a suitable summation technique. The order of the Padé approximants must be selected such that the entropy is directly proportional to α_T at low temperatures, which restricts us to $[N+1,N]$ approximants for the temperature in terms of entropy. The specific heat could then be obtained by differentiating the temperature with respect to entropy and then inverting. In order to allow comparison with previous work, the results were normalized to the mean-field theory discontinuity, so that if at low temperatures the specific heat achieved the mean-field value, the normalized specific heat would be unity.

We will describe as "unconstrained" those approximants where the only information supplied is the series and the order of the approximant. The constrained approximants have the further requirement that they must tend to the mean-field limit at low temperatures. This is imposed using the method of Hikami and Fujita [Eq. (2.16)]. In our case the mean-field limit is $\alpha_T = s/\beta_a$, which becomes the requirement that $a_{N+1} + b_N\beta_a = 0$.

We also make comparisons with the best previous method where the $[N,N]$ Padé-Borel approximant for the free-energy series in x is constrained as in Eq. (2.16), with an additional factor of 2^N removed from the coefficients of the series. (See Ref. 8 for the justification of this factor 2^N.)

Examination of Fig. 3 for the entropy shows that the skeleton-graph series fits the Monte Carlo data slightly better than the original method, but in itself this would not justify the extra effort of determining the skeleton-

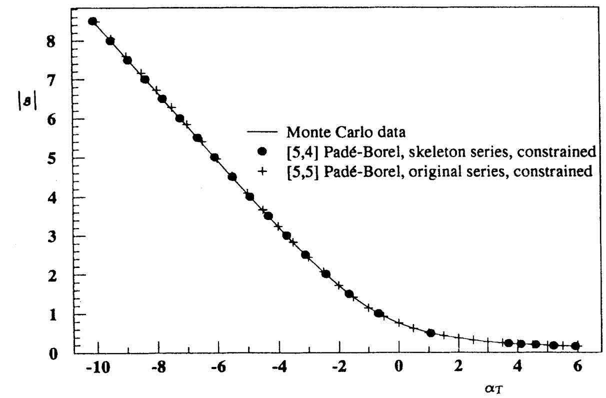

FIG. 3. Entropy data for the two-dimensional case, showing that the constrained Padé-Borel approximant constructed from the skeleton-graph expansion fits the Monte Carlo data slightly better than that similarly constructed from the original series.

graph expansion. The significant improvement is in the manner that the unconstrained Padé-Borel results hang together and yield the correct characteristic curve of Fig. 4. In fact the difference between unconstrained and constrained Padé-Borel approximants of the same order is only apparent below $\alpha_T \approx -2$ (Figs. 4 and 5).

The difference between the Padé-Borel approximants and the Monte Carlo data decreases in the order [4,3], [3,2], [6,5], [5,4]. Thus there is an odd-even effect associated with how the accuracy improves with N. (A possible explanation can be found in the stability of the Padé forms themselves. For the Padé forms with odd-order denominators the positions of the poles and the values obtained from the approximants are far more sensitive to small changes in the coefficients of the perturbation series.)

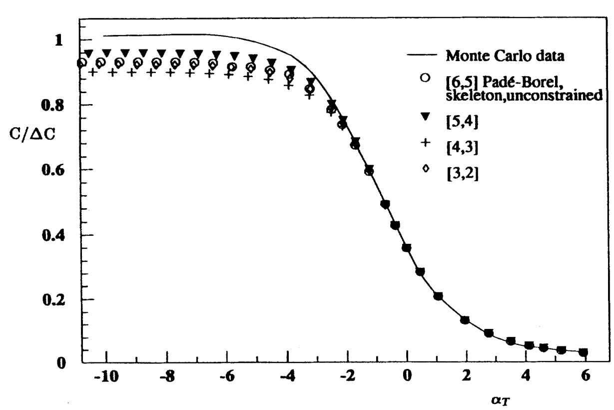

FIG. 4. Comparison of different orders of unconstrained Padé-Borel approximants of the skeleton-graph series for the specific-heat function. (Because of numerical differentiation problems the Monte Carlo data should only be treated as an aid to the eye.)

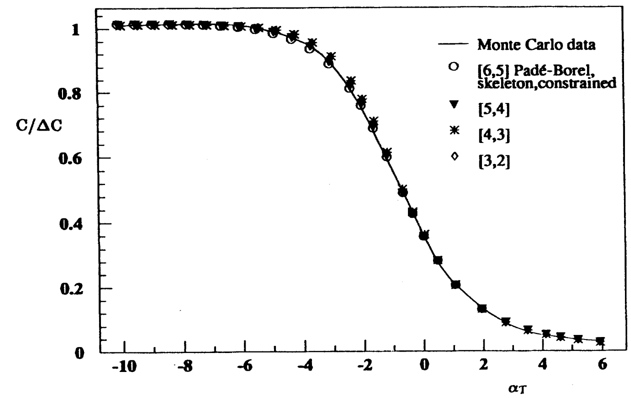

FIG. 5. Same as Fig. 4, but using the constrained approximants.

The Padé approximants were also evaluated (see Fig. 6), and we again find that without the constraint, although the shape of the curve is similar to the Monte Carlo data, the low-temperature limit is different, the difference being greater than that between the Monte Carlo data and Padé-Borel approximants. Unlike the latter the Padé approximants do not exhibit an odd-even effect with increasing order.

B. Three-dimensional case

In this case we again find that if we do not impose a low-temperature limit the value of the specific heat at low temperatures is very dependent on the approximation method used. The curves produced using the skeleton-graph series with both Padé and Padé-Borel approximants are smooth with no peaks. However, as pointed out by Hikami, Fujita, and Larkin[7] there is a peak in the Padé approximant if it is constructed from the original series, see Fig. 7.

They provided evidence for a transition by the calculation of the Abrikosov factor (β_a) from the free-energy

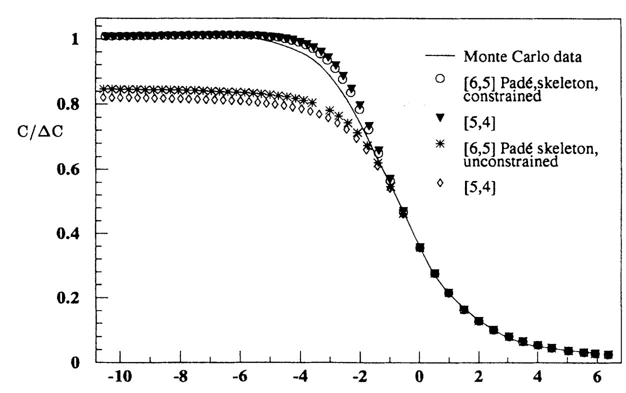

FIG. 6. Comparison of different orders of Padé approximants constrained and unconstrained for the specific-heat function for the two-dimensional case.

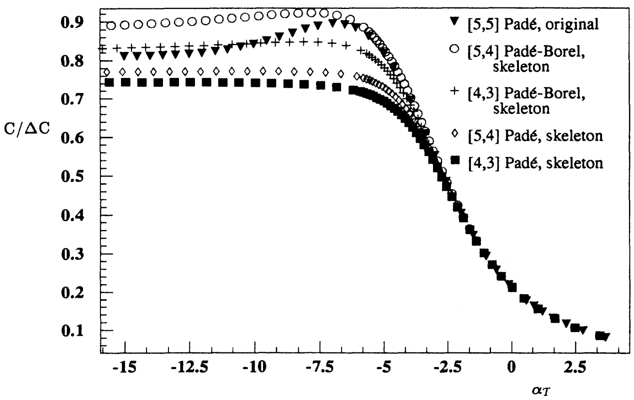

FIG. 7. Specific-heat data for the three-dimensional case. We find that the low-temperature limit, as in the other dimensions, depends on the approximation used. It is only the Padé approximant constructed from the original series that has a pronounced peak.

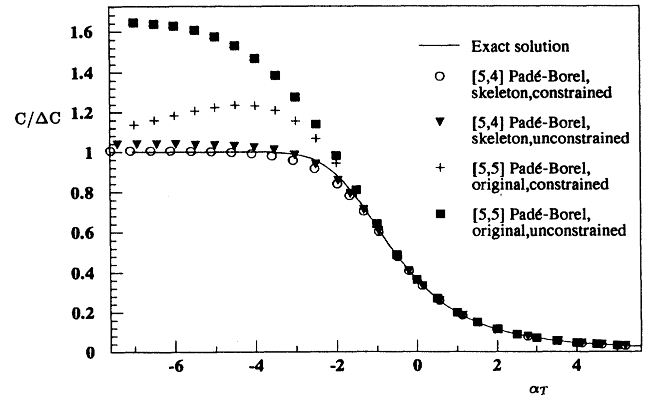

FIG. 8. Specific-heat function for the toy model demonstrating that the skeleton-graph expansion gives a more convincing approximation than the original series to the exact answer.

perturbation series in x reexpressed in a simple $[N, N-1]$ Padé form. In two dimensions if these values are plotted against $1/(N-1)^2$, the value of β_a for $N \to \infty$ is close to the standard answer of $\beta_a = 1.16$. They subsequently applied this technique to the three-dimensional case, and using two of the three points available, obtained $\beta_a = 1.28$, which if true would indicate a phase transition, i.e., $\beta_a \neq 1.16$ is explained by the presence of a phase transition. However, if all three points are used (with the value of β_a corrected for the [3,2] to 1.667) and plotted against $1/(N-1)$, these extrapolate to $\beta_a \approx 1.17$, which does not indicate a phase transition.

Trying to perform a similar analysis for the skeleton-graph series is tricky, since in two dimensions the Padé-Borel approximants do not have uniform convergence (as discussed in Sec. IV A), and the Padé approximants do not fit a simple $1/N^m$ form. However, for the former only an abscissa of $1/N$ allows both lines to have an infinite N limit of approximately 1.16.

We can only conclude that the existence of a phase transition in three dimensions cannot be reliably ascertained through analysis of the existing series alone.

C. Toy model

The results for the two-dimensional case appeared very encouraging, so the skeleton-graph technique was also applied to the toy model, leading to the results shown in Fig. 8. Unfortunately, it was found that although the results were promising for the [5,4] Padé-Borel approximant—it has the correct curve shape and a low-temperature limit of 1.03—the higher order approximants do not home in on the correct low-temperature limit, with values oscillating around 1.1 (Fig. 4). Using a simple Padé approximant the convergence of the curves was found to be monotonic, but very slow. The Padé approximants are easy to calculate, so we have evaluated them up to [22,21] order (Fig. 9). The convergence looks good up to [15,14]. Unfortunately, above this order all approximants overshoot the exact answer, first doing so at $y \approx -3$.

In previous papers the specific-heat curves have been constrained such that at low temperatures the correct result is obtained. This works well for the [5,4] Padé-Borel approximant but appears to make the approximants unstable at higher orders.

From the exact solution for the free energy, Eq. (2.23), we know that it contains '$w(iy/\sqrt{2})$'. Examination of Abramowitz and Stegun[18] [Eq. (7.1.4)] shows that there exists an integral representation

$$w\left(\frac{iy}{\sqrt{2}}\right) = \frac{y}{\pi\sqrt{2}} \int_0^\infty dt \, \frac{e^{-t}}{\sqrt{t}(t+y^2/2)}, \quad \Re y > 0. \tag{4.1}$$

This suggested that possibly there should be a square root in the denominator of the integrand, rather than a straight Borel resummation. Hence the Borel integral was modified such that it had a $1/\sqrt{t}$ singularity in the integrand, but this did not significantly affect the specific-heat function obtained.

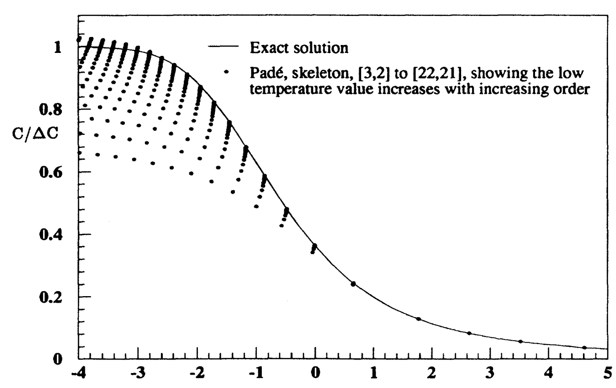

FIG. 9. Unconstrained Padé approximants for the toy model up to [22,21] order, showing that they do not converge to the correct low-temperature value.

Despite their faults the approximants derived from the skeleton-graph series are a vast improvement on those obtained from the original series. The latter in both the Padé and Padé-Borel forms do not exhibit the correct shape for the exact answer or the low-temperature limit; e.g., the [5,5] Padé-Borel approximant has a limit of 1.5. Constraining the curves only serves to produce a hump in the curves, which gets worse with increasing order.

These results suggest that extrapolation of the skeleton-graph series is more reliable than that of the original series. They also indicate that a wrong low-temperature limit can be an artifact of the resummation procedure.

D. Analysis of the toy model and relevance to higher-dimensional cases

From the previous section it is obvious that approximating the toy model is in itself not a trivial task. It was hoped that gaining an insight into the underlying problems associated with the toy model would help our understanding of the two-dimensional case.

We know that all the approximation methods work well for $y \geq 0$, i.e., above the mean-field transition temperature, but collapse in varying degrees for $y < 0$. Examination of the exact solution shows us why, at least for the standard perturbation theory. Consider the free energy [Eq. (2.23)] in conjunction with the expression for $w(iy)$ [Ref. 18, Eq. (7.1.11)],

$$w(-iy) = 2e^{y^2} - w(iy); \tag{4.2}$$

on passing through $y = 0$ an exponential term switches in, which is not picked up by normal perturbation theory. For $y < 0$, the argument of the exponential in the integral of Eq. (2.20) has a maximum at $t = 0$ and minima on either side. The exponential contribution comes from the maximum.

It is possible that the difference between the Monte Carlo data and the unconstrained skeleton-graph Padé and Padé-Borel approximants in the two-dimensional case is also due to saddle-point contributions that are only a finite-energy difference away from the point about which we perturb. They could be provided by the finite-energy solutions which we shall show exist in the two-dimensional case. These contributions are not picked up by the perturbation expansion and hence may prevent us resumming the series to give the correct result.

In two dimensions the existence of finite energy solutions can be shown starting with the Landau-Ginzburg equation (2.1). The order parameter when truncated to the lowest Landau level can be represented by[13]

$$\psi(z) = \left(\frac{\Phi_0}{\beta L_z B}\right)^{\frac{1}{4}} \sum_{m=0}^{\infty} v_m \psi_m(z) = \left(\frac{\Phi_0}{\beta L_z B}\right)^{\frac{1}{4}} e^{-zz^*/(4P)} \sum_{m=0}^{\infty} g_m v_m z^m, \tag{4.3}$$

where $g_m = (\pi m!)^{-1/2}(1/2P)^{(m+1)/2}$, $P = \Phi_0/(2\pi B)$ with Φ_0 the flux quantum and $z = x + iy$ such that $\{z_i\}$ are the (complex) positions of the vortices.

The free-energy functional can now be written in terms of the complex expansion parameters $\{v_m\}$,

$$F[\{v_m\}]/kT_c = \alpha_T \sum_{m=0}^{\infty} v_m v_m^* + \sum_{m,p,n,r=0}^{\infty} \frac{(m+p)!\, v_m v_p v_n^* v_r^*}{(m!p!n!r!)^{1/2}\, 2^{m+p+2}}\, \delta_{m+p,n+r}\, . \tag{4.4}$$

If we consider the simplest solution of no vortices present, that is, $v_0 = c_0$, then

$$F/kT_c = \alpha_T c_0^* c_0 + c_0^{*\,2} c_0^2. \tag{4.5}$$

If we minimize this with respect to c_0 then we obtain $c_0^* c_0 = -\alpha_T/2$, and provided $\alpha_T < 0$ we have $F/kT_c = -\alpha_T^2/4$, a finite-energy solution. Similar solutions can be found for any number of vortices present. All these solutions are saddle-point solutions, that is, they are unstable against the addition of further vortices.

In three dimensions we have been unable to find any finite-energy stationary points. This could mean that the series is convergent in three dimensions after Padé-Borel resummation.

V. ALTERNATIVE SERIES EXPANSIONS OR RESUMMATIONS

In this section we detail two alternative methods that have been tried out on the toy model in an attempt to find one that converges to the known exact answer: the δ expansion, which although known to converge was found to be very slow, and the Stevenson transformation, which only converges to the correct answer above the mean-field transition temperature.

A. The δ expansion

The δ expansion is a method which has been proven recently by Buckley, Duncan, and Jones[10] to produce a convergent series. They had applied it to a toy model similar to our own, i.e.,

$$I = \int_{-\infty}^{+\infty} \exp[-\mu^2 x^2 - g x^4]\, dx; \tag{5.1}$$

cf. the integral of Eq. (2.21). The δ expansion is not a new technique, but they had shown that the expansion converged exponentially fast, with the non-perturbative terms being picked up. That is, it worked in the low-temperature regime $\mu^2 < 0$. This seemed ideally suited to our problem, for it is the low-temperature regime which is of most interest.

The δ expansion begins by rewriting the exponential in Eq. (2.20) as

$$\exp[-(1-4x)t-x^2t] \Rightarrow \exp\{-\lambda t+\delta[-xt^2+(\lambda-1+4x)t]\}; \tag{5.2}$$

δ is our new expansion parameter and λ is another artificial parameter. To obtain a series approximation we expand down the δ part of the exponential, then expand again using the binomial theorem and integrate over t:

$$f_{0\mathrm{D}} = -\ln\left[\sum_{n=0}^{\infty}\delta^n \sum_{r=0}^{n} \frac{(\lambda-1+4x)^{(n-r)}(-x)^r(n+r)!}{r!(n-r)!\lambda^{n+r+1}}\right]. \tag{5.3}$$

To consider a particular order of δ, say, k, we simply stop the sum over n at k and then set $\delta = 1$; this is the partial sum for $f_{0\mathrm{D}}$ up to k and is denoted by $\{f_{0\mathrm{D}}\}_k$. The coefficients in the series can be calculated simply using MATHEMATICA. The next step requires the optimization of λ, which is done by invoking the principle of minimum sensitivity (PMS). This in essence requires that the dependence of $\{f_{0\mathrm{D}}\}_k$ be minimized. The necessary condition is

$$\frac{d\{f_{0\mathrm{D}}\}_k}{d\lambda} = 0. \tag{5.4}$$

For all but the lowest orders the PMS equation for general x becomes too large to solve analytically. Thus the PMS condition was solved for chosen values of x, such that we had a discrete set of values for $f_{0\mathrm{D}}$. The specific heat was then obtained by numerical differentiation. Values of x were chosen such that the error due to the numerical differentiation was $\sim 10^{-4}$.

For our toy model, solutions to the PMS equation only exist for odd orders in δ. Even-order values could be calculated using a more complicated PMS condition, but as this was only a trial of the method sufficient information could be obtained just from the odd orders. The δ expansion was only calculated up to 11th order, chosen because our two-dimensional series has 11 terms. Up to 9th order, the PMS condition could be solved directly using MATHEMATICA. For the 11th order, a Newton-Raphson approach was used; the initial value of λ chosen for each x was that calculated at 9th order.

The results for the specific heat in the region $y > 0$ were extremely accurate, with the only limitation being the numerical differentiation, even at 5th order, for $y = 4$. However, the results were less impressive in the $y < 0$ region. Only the 9th and 11th order approximations gave any results of the correct sign in this region, before fluctuating wildly and then producing imaginary values around $y = -2$. Thus although it has been proved that this method converges, it requires rather more than 11 terms to even get an idea of what is happening at low temperatures.

B. Stevenson transformation

This is a simpler, earlier use of the PMS constraint than the δ expansion. Along with a very simple transformation of variable it has been shown to produce good results in such cases as the alternating factorial series, which has zero radius of convergence. Stevenson states that for a given series "if we optimize the choice of τ (the PMS parameter) at each order the resulting sequence of approximations is convergent,"[11] although not necessarily to the exact function.

The method was tried on the toy although there were no technical complications in transferring it to the two-dimensional case. If we consider the skeleton-graph series then the suggested transformation is

$$s = \tilde{s}/(1-\tau\tilde{s}), \tag{5.5}$$

where $\tilde{s}$ is our new variable and τ is the PMS parameter. This new variable is substituted into Eq. (3.6), and the equation is expanded out, to the selected order. For example, the third-order approximant (where order is determined by the power of $\tilde{s}$) is

$$y(\tilde{s},\tau) = -1/\tilde{s} + 2\tilde{s} + 2\tilde{s}^3 + (1+2\tilde{s}^2-6\tilde{s}^4)\tau + 2\tilde{s}^3\tau^2. \tag{5.6}$$

This is then minimized with respect to τ to give several values of τ. As it was unclear which value to choose and the exact answer is known all values were substituted back into Eq. (5.6) to find the value with the answer closest to the exact answer. It was evident from this that the most negative value of τ was appropriate.

To avoid having to numerically differentiate, comparison was made directly between the value of y obtained for a given s with that for the exact answer. Good results were obtained for $y \geq 0$, but no sensible values were obtained for $y < 0$, even up to 24th order.

VI. EXPERIMENTAL DATA

It is apparent from the methods detailed in the previous sections that starting from the perturbation series there are still problems in extrapolating to the low-temperature regime. The skeleton-graph expansion is an improvement but does not converge to the correct limit when resummed by Padé or Padé-Borel techniques for the toy model. We expect similar problems for the two-dimensional case, but in practice the constrained [5,4] Padé-Borel approximant is an excellent fit to the Monte Carlo data.

With this proviso, how do our theoretical results compare with those obtained experimentally? In the real world we can only approximate to a two-dimensional system. Urbach *et al.*[12] have done this by investigating the specific-heat properties of a multilayer system of superconducting $Mo_{77}Ge_{23}$ separated by insulating amorphous germanium.

In order to avoid resummation problems, we will compare the experimental results with the Monte Carlo data. The comparison is disappointing (Fig. 10), making the differences between the various resummation results appear insignificant. Although noisy, at least for high temperatures there is some agreement—but at low temperatures the shapes of the curves and their values are completely different. In fact the zero-dimensional specific-

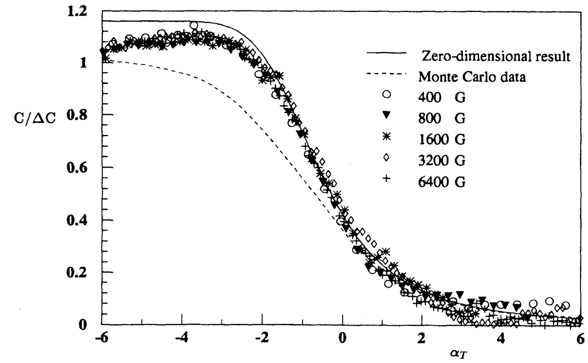

FIG. 10. Comparison of the experimental data of Urbach *et al.* (Ref. 12) with the two-dimensional Monte Carlo data and the exact zero-dimensional solution. The zero-dimensional data have been multiplied by the Abrikosov factor, $\beta_a \approx 1.16$.

heat curve is a better fit around T_c.

It is not known whether the source of the discrepancy is theoretical, experimental, or both. One possibility is that the theoretical model does not take into account disorder, and this is being investigated at present using Monte Carlo simulations. There is also the problem that the sample is not really two dimensional so that the whole of the Landau-Ginzburg expression of Eq. (2.1) applies to it. Although each of the layers can be considered two dimensional, the measured specific heat is an average of all the layers, which are coupled via the electromagnetic field. One would expect that the theory of this situation would be dependent on the thickness of the layers *and* their spacing.

VII. CONCLUSIONS

We have used the conventional perturbation series for thin-film superconductors to study the specific heat in the low-temperature region. For this special case we have been able to improve upon the standard extrapolation techniques. By noting that the renormalized propagator (the entropy) is directly proportional to the bare propagator, we were able to rewrite the available series in terms of the renormalized propagator. Having reformulated the series we could then use the standard Padé and Padé-Borel techniques to extrapolate it to the low-temperature region.

The specific-heat function evaluated by this technique differs detectably from the Monte Carlo results if it is not constrained by the mean-field low-temperature limit. A possible source of the discrepancy between the Monte Carlo and the series extrapolation has been found through study of the zero-dimensional toy case, which is exactly soluble. The skeleton-graph expansion works significantly better than the original series for this problem, although it does not converge after resummation, either by Padé or Padé-Borel methods, to the correct low-temperature limit. In the toy problem it is found that problems arise because of an exponential term which switches in below the mean-field transition temperature—it is in fact a contribution from the saddle point in the potential. In order for a similar argument to be applied in the two-dimensional case we require there to be finite-energy solutions, and the existence of such solutions has been demonstrated.

In three dimensions the inversion of the series does not correspond to an expansion in terms of skeleton graphs. However, the series has been inverted and reveals no strong evidence for a phase transition.

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