Phase boundary of superconducting networks: A new approximation scheme

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We calculate the normal-superconducting phase boundary of a superconducting wire network in arbitrary magnetic fields using the London approximation of the linearized Ginzburg-Landau equation. Our formulation in terms of the constituent loop currents allows an iteration procedure to calculate the energy of a network, which in turn determines the mean-field transition temperature $T_c(H)$. For infinite lattices, finite-order truncation in this scheme produces good agreement with other calculations and experiments.

There has been substantial activity over the past few years in the study of the behavior of superconducting networks in an external magnetic field. The importance of the effects of frustration due to lattice geometry has been clearly seen in the superconducting phase boundary $T_c(H)$ or magnetoresistance near $T_c$ of many experimental systems. $T_c(H)$ has been calculated numerically for many of these networks by solving the linearized Ginzburg-Landau (GL) equation. Although these calculations agree with the experimental results quite well, it is not easy to develop simple physical insights from these calculations. For example, the ground-state fluxoid distributions in an arbitrary external field cannot be easily obtained. Previously, the ground-state fluxoid distributions of the infinite-square lattice have been obtained by using the two-dimensional $XY$ model appropriate for arrays of Josephson junctions with their sinusoidal current-phase relation. The essential physics of the networks in a magnetic field is contained in the phase information through the fluxoid quantization requirement, consistent with the current conservation. To that extent, the constant-amplitude approximation (the London approach) of the GL equation is adequate in the description of the networks. While mathematically simpler, it enables us to investigate more complex networks. Note that the London approach is also equivalent to the $XY$ model in the limit of small phase differences between nodes.

Using the London approach, de Gennes proposed a loop-current formalism to calculate the magnetic susceptibility of finite clusters in small fields. Subsequently, Stephen considered an equivalent resistance network to calculate the susceptibility of the (fractal) Sierpinski gasket. Alexander and Halevi have further elucidated this picture and discussed the local critical currents of superconducting clusters in finite fields. In this article, we show that the flux quantization requirement of a network leads to a simple formula for the total energy in an arbitrary magnetic field, in which the fluxoid distribution is the input parameter. Ground-state energies and ground-state fluxoid configurations are obtained by the minimization of the total energy. Furthermore, we show that this formalism allows a natural infinite series expansion. Low-order truncations often lead to very good approximations of the superconducting phase boundary of an infinite network. We use the well-studied infinite square network as the testing ground to illustrate the usefulness of this expansion. We also present theoretical results for a complex periodic network.

In the London limit, the GL free energy for superconducting networks is

$$\delta F_s = \sum_{\langle ij \rangle} l_{ij} \left[ \alpha_{ij}^2 - \frac{1}{\xi^2} \right] |\Delta|^2 + \frac{b}{2} |\Delta|^4 , \quad (1)$$

where

$$\alpha_{ij} \equiv \frac{\partial \varphi_{ij}(s)}{\partial s} - 2\pi A_{ij}(s)/\Phi_0 ,$$

$L_{ij}$ is the bond length between nodes $i$ and $j$, $\varphi_{ij}(s)$ is the phase of the order parameter, $A_{ij}(s)$ is the tangential vector potential, and $\Phi_0$ is the superconducting flux quantum. Since $\alpha_{ij}$, the gauge-invariant phase gradient, is simply proportional to the supercurrent in the bond, the two names will be used interchangeably. The mean-field $T_c$ is obtained when the coefficient of the $|\Delta|^2$ of Eq. (1) vanishes:

$$\left[ \frac{a}{\xi} \right]^2 \left( \frac{T_c(H)}{T_c(0)} - 1 \right) = \frac{\sum_{\langle ij \rangle} l_{ij} \alpha_{ij}^2}{\sum_{\langle ij \rangle} l_{ij}} \equiv \frac{U}{\Lambda} , \quad (2)$$

where $a$ is the characteristic bond length of the network. In Eq. (2) and the rest of this paper, $l_{ij}$ and $\alpha_{ij}$ are redefined to be in units of $a$ and its inverse, respectively. $U \equiv \sum_{\langle ij \rangle} l_{ij} \alpha_{ij}^2$ can be thought of as the total energy of the network, and the reduction of the normalized $T_c$ is proportional to the energy per bond, $U/\Lambda$, with $\Lambda$ being the total bond length of the network, i.e., $\sum_{\langle ij \rangle} l_{ij}$.

In the loop-current formalism the total energy can be written as

$$U = \sum_m L_{mm} \alpha_m^2 - \sum_{mn} l_{mn} \alpha_m \alpha_n = \alpha^\dagger (L - 1) \alpha , \quad (3)$$

where $\alpha_m$ refers to the phase gradient or current in loop $m$, $l_{mn}$ is the length of the bond separating the adjacent
loops $m$ and $n$, and $L_{mn} = \sum_n l_{mn}$ is the circumference of loop $m$. The sums over $m$ and $n$ are unrestricted. The last part of Eq. (3) is simply the matrix form of the same expression, where $\alpha$ is a state vector representing the gauge-invariant loop-current configuration, $\alpha^T$ its transpose, $L$ is the diagonal matrix of $L_{mn}$, and $l$ is a symmetric matrix with its nonzero elements defined by the bond length separating the adjacent loops. To calculate the ground-state energy and the resulting $T_c$, one needs to find the ground-state vector $\alpha$, which is required to satisfy the fluxoid quantization condition:

\[
(L - l)\alpha = L\alpha^{(0)},
\]

(4)

with

\[
\alpha^{(0)} = 2\pi L^{-1}(\Phi - N),
\]

(5)

where $\Phi$ is the vector representing the applied flux in the loops in units of the flux quantum $\Phi_0$ and $N$ is the corresponding vector of fluxoid quantum numbers in the loops. We call $\alpha^{(0)}$ the bare loop current because it would be the actual current if the loop $m$ were not interacting with the other loops. $\Phi$ is uniquely determined by the externally applied field and the loop areas, thus $\alpha^{(0)}$ is known subject to the fluxoid distribution $N$. The actual loop currents, $\alpha'$ can be obtained in terms of the bare loop current from Eq. (4)

\[
\alpha' = (L - l)^{-1}L\alpha^{(0)}.
\]

(6)

Substituting Eq. (6) into Eq. (3), we have

\[
U = \alpha^{(0)}^T L (L - l)^{-1}L\alpha^{(0)},
\]

(7)

or equivalently,

\[
U = (2\pi)^2 (\Phi - N)^T (L - l)^{-1}(\Phi - N).
\]

(7a)

For finite networks in the small-field limit, i.e., $N = 0$, Eq. (7a) reduces to the one obtained by de Gennes and by Stephen. For infinite networks or finite networks in finite fields, the nonzero fluxoids play an important role in determining their magnetic-field effects, which has been discussed in some detail by Alexander and Halevi without explicitly using Eq. (7a). For relatively small networks, inverting the matrix $(L - l)$ is simple and straightforward. Then both ground-state fluxoid distribution and ground-state energy for an arbitrary field can be obtained easily. However, for very large or infinite networks, inverting the matrix becomes much more difficult. It is particularly so if the network is nonperiodic. We show that a good approximation of the energy $U$ can be obtained by using an infinite series expansion in terms of powers of $l$ instead of the matrix inversion. To simplify discussion, let us consider only infinite networks in the following.

The formalism becomes simpler if we rescale $\alpha$ and $l$ as $\bar{\alpha} = \sqrt{L} \alpha$ and $\bar{l} = (1/\sqrt{L}) l (1/\sqrt{L})$, respectively. An interaction potential of the loop currents can be defined as

\[
\bar{v} = \frac{1}{1 - \bar{l}},
\]

(8)

which is independent of the external fields. Then the loop-current distribution can be rewritten as $\bar{\alpha} = v \bar{\alpha}^{(0)}$ where $\bar{\alpha}^{(0)}$ is the rescaled bare loop-current distribution. Likewise the total energy $U$ can be rewritten as

\[
U = \bar{\alpha}^{(0)^T} \bar{v} \bar{\alpha}^{(0)} \equiv U_S \langle \bar{v} \rangle.
\]

(9)

Hereafter we use $\langle (A) \rangle$ to represent the average value of the matrix $A$ with respect to the bare loop-current vector. $U_S = \bar{\alpha}^{(0)^T} \bar{\alpha}^{(0)}$ is the energy of the network if the mutual interactions among the current loops are ignored. It is easy to prove that the eigenvalues of $\bar{l}$ are bounded by $-1$ and $1$. As a matter of fact, $1$ is always an eigenvalue and the corresponding eigenvector is $\sqrt{L} \mathbf{1}$, where $\mathbf{1}$ is the vector of $1$'s. It is obvious from Eq. (8) that the energy $U$ is infinite if $\bar{\alpha}^{(0)}$ has a finite projection onto this eigenvector of $\bar{l}$. To avoid this situation, every physical fluxoid distribution must be orthogonal to this state. This is equivalent to a sum rule that requires the sum of the applied flux in units of $\Phi_0$ to be equal to the sum of the fluxoid numbers:

\[
\sum_m \Phi_m = \sum_m N_m.
\]

(10)

The sum rule requires a nonzero fluxoid distribution for an infinite network even in the small-field limit. This is the reason for the linear field dependence of $T_c$ near zero magnetic field. This intuitively understandable constraint on infinite networks is formally equivalent to the global charge neutrality condition for a Coulomb gas. Furthermore, we expect that the ground-state or low-energy states also satisfy an approximate local sum rule, which can be used to ease the search for ground-state energies.

There are many ways to expand $\bar{v}$ in powers of $l$. In the following, we determine an expansion scheme that leads to a particularly good approximation for the energy $U$.

\[
\frac{1}{1 - l} = \frac{1}{1 - c} \left(1 - \frac{l - c}{1 - c}\right)^{-1} = \frac{1}{1 - c} \sum_{k=0}^{\infty} \left(\frac{l - c}{1 - c}\right)^k,
\]

(11a)

where $c$ is an arbitrary constant. If $c$ is negative, the series in Eq. (11) converges for any physical state because the eigenvalues of $\bar{l}$ are bounded between $-1$ and $1$. For evaluating $U$, the choice of $c = \langle \bar{l} \rangle$ appears to give the best result. The minimization of $U$ automatically restricts $\langle \bar{l} \rangle$ in the range of $-1$ and $0$ for many networks we have considered. With this choice, Eq. (11) can be rewritten as

\[
U = U_S \left(\frac{1}{1 - \bar{l}}\right) = \frac{U_S}{1 - \langle \bar{l} \rangle} \sum_k \left(\frac{\bar{l} - \langle \bar{l} \rangle}{1 - \langle \bar{l} \rangle}\right)^k.
\]

(11b)

The $k$th term in the series is related to the $k$th moment of the operator about its average value. Let us define $U_n$, the $n$th order approximation of $U$, to be the finite summation in Eq. (11b) up to $k = n$. Note that $U_1 = U_S / (1 - \langle \bar{l} \rangle)$, which will be referred to as the first-order approximation.

We consider the infinite-square lattice as an example to illustrate the use of Eq. (11b). Let $\bar{f}$ be the average fluxoid number per loop. Equation (10) requires $f$ to be equal
to the applied flux per loop $\Phi$. For this example, it is
sufficient to calculate the energy per bond, $U/\Lambda$, in the
range of $f$ from 0 to $\frac{1}{2}$ because the ground-state energy
as a function of $f$ is a periodic function of period 1 and is
symmetric about $f = \frac{1}{2}$. For a given $f$, the number frac-
tions of the loops with one fluxoid quantum and zero
fluxoid quantum are $f$ and $(1-f)$, respectively. To
calculate the first-order energy $U_1$, we need to obtain $U_5$
and $\langle T \rangle$. $U_5/\Lambda$ depends only on the total fluxoid num-
ber. Thus it is easily obtained by applying the sum rule:

$$\frac{1}{\Lambda}a^{(0)(f)}a^{(0)} = \frac{(2\pi)^3}{8}[f(f-1)^2 + (1-f)f^2]$$

$$= \frac{\pi^2}{2} (f-f^2).$$

(12)

$\langle T \rangle$ can also be easily calculated by noting that it is ener-
ggetically favorable to pair opposite loop currents as the
nearest neighbors. It is easy to see that the minority
loops (loops with one fluxoid) can always have majority
loops (loops with zero fluxoid) as neighbors. That takes
care of $4f$ nearest-neighbor pairs per loop. The remain-
ing, $2-4f$, must be the pairs of majority, i.e., “zero-zero”
pairs. Thus we have

$$\frac{1}{\Lambda}a^{(0)(f)}a^{(0)} = \frac{(2\pi)^2}{4^2}[4f(f-1)f + (2-4f)f^2]$$

$$= \frac{\pi^2}{4} (-2f^2).$$

(13)

To calculate the energy to the second order, we also need
$\langle T^2 \rangle$, which represents the interactions of loop currents
with their second nearest neighbors. A calculation of
$\langle T^2 \rangle$ based on a hierarchical energy consideration of in-
teracting pairs of loop currents will be published else-
where.\footnote{It is sufficient to mention here that the resulting
$\langle T^2 \rangle$ is a piecewise analytic function of $f$ with cusplike
structures at $f = \frac{1}{3}$ and $\frac{2}{3}$. The calculated $U_1/\Lambda$
and $U_5/\Lambda$ are presented in Fig. 1(a). To check the con-
vergence, we also plot some exact values as open circles in
Fig. 1(a), calculated for a few simple rational values of $f$.
The general excellent agreement between the exact values
and the first- and second-order results demonstrates the
success of the proposed expansion scheme and its use-
fulness for calculating an approximate $T$, in arbitrary
fields. Note that our results represent a systematic piece-wise
analytical approximation of the phase boundary. The
previous analytical approximation obtained by Tinkham
et al.,$^1\frac{1}{11}$ predicts a cusplike structure at $f = \frac{1}{2}$ only.
Behrooz et al.$^1\frac{1}{12}$ have also obtained a simple analytic
approximation equivalent to our $U_5/\Lambda$, Eq. (12), which has
no structure at $f = \frac{1}{2}$.

We expect to have more cusplike structures at other
rational numbers of $\Phi$ by including higher-order terms,
which involve interactions at larger distances. They are
much less pronounced, and experimentally much more
difficult to resolve. In Fig. 1(b), the experimental data of
Pannetier et al.$^1\frac{3}$ is shown together with our second-order
calculation. We emphasize that there is no adjustable pa-
rameter in this plot because both $\alpha$ and $\xi^{(0)}$ were
measured experimentally. Except for the slope near zero or
integer flux quantum, the second-order curve fits the data
quite well. The discrepancy of the low-field slope be-
tween the data and our calculations is due to the inade-
quacy of the London approximation rather than our ap-
proximation for the energy calculation. It is to be expect-
ed because, in low fields, the phase gradient needed to
enclose a flux quantum is too large for a single loop to sus-
tain the superconducting state, i.e., some bonds have to
be driven normal near the phase boundary to lower the
total energy. For $f$ near $\frac{1}{2}$, the London approximation
is much better because the magnitude of the order param-
eter is much more uniform.$^{13}$

Although higher-order calculations are needed to re-
veal fine structures on the phase boundary of the infinite-
square network, the first-order result is already adequate
to predict the overall magnitude and the most prominent
features as shown in the previous example. To illustrate
this point further, we calculate the phase boundary of a
complex periodic network with the space-group symme-
try $P4gm$, studied in Ref. 14. This network consists of
two shapes, equilateral triangles and squares. Since the
sum rule requires only the sum of the fluxoid numbers in
the two shapes be fixed by the external field, the energy
for noninteracting loop currents $U_5$ is obtained from a
simple one-parameter minimization. To obtain $U_5$, it is
sufficient to know that the $P4gm$ lattice has four triangles
two squares per unit cell. To calculate $U_1$, we need
to know that there are zero square-square, two triangle-
triangle, and eight triangle-square nearest neighbors per
unit cell. With these as the input parameters we have ob-
tained an approximate semianalytical expression$^9$ for $U_1$
in terms of the average fluxoid numbers in the two
shapes. The minimization of $U_1$ is done similar to that of
$U_5$. The results for both $U_5/\Lambda$ and $U_1/\Lambda$ are presented

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Normalized $T_c(\Phi)$ as a function of applied flux per
loop for an infinite-square lattice. (a) The results of the loop-
current formalism: Solid line is the second-order results and the
dashed line is the first-order results. Circles are the exact results
within the London approach at $\Phi=0$, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$,
$\frac{1}{3}$, $\frac{2}{3}$, $\frac{5}{8}$, $\frac{7}{8}$, and their symmetric points about $\frac{1}{2}$.
(b) Comparison to experiment: Solid line is the second-order pre-
diction of the loop-current formalism; dotted line is the experimen-
tal data of Pannetier et al. (Ref. 4). There are no adjustable parameters.}
\end{figure}
FIG. 2. Normalized \( T_c \) as a function of the applied flux in the triangle. (a) Theoretical calculation by Nori and Niu (Ref. 15) (b) Loop-current formalism: The dotted line is \( U_5 / A \) and the solid line is the first-order result, \( U_1 / A \). (c) The average fluxoids numbers in the square and the triangle from the first-order calculation.

in Fig. 2(b) as dotted and solid lines, respectively. For comparison, the numerical GL result by Nori and Niu\(^{15}\) is shown in Fig. 2(a). There are no adjustable parameters in all three calculations. Note that all three curves are similar, particularly near the major energy minima \( (T_c \text{ maxima}) \). This implies that the interactions between loop currents are relatively unimportant in these regions. The effect of interaction is most prominent near the energy maxima, where the lattice is more frustrated. The semi-quantitative agreement between our first-order calculation and the GL result is particularly impressive. The GL result is probably more accurate where the two differ, but our first-order energy is much simpler to obtain. The present model also predicts the average fluxoid numbers in the ground state, which has not been obtained previously. The average fluxoid numbers in the triangular and square loops obtained for the first-order calculation are shown in Fig. 2(c). It is clear from Fig. 2(b) and 2(c) that the major dips of the energy curve occur when the fluxoid in the triangle is an integer. This is because the frustration in the triangle (compared to the square) costs more energy and there are more triangles in the network. Figure 2(c) is in total agreement with the previous exact results\(^{14}\) calculated only at some discrete field values. We note that, since only the average numbers of shapes and nearest neighbors are needed, the first-order calculation can be carried out even for nonperiodic lattices with equal ease.\(^{9}\)

In conclusion, we have demonstrated that an expansion scheme in terms of nearest-neighbor connection matrix can be used to calculate the phase boundary of superconducting networks in arbitrary fields without extensive numerical computation. Energy can be easily calculated for different fluxoid distributions. This approach is particularly useful for complex lattices.

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\(^{1}\)For a recent review, see the Proceedings of the NATO Advanced Research Workshop on Coherence in Superconducting Networks, Delft, 1988 [Physica, B 152, 1 (1988)].


\(^{9}\)C. C. Chi, P. Santhanam, and P. E. Blöchli (unpublished).

\(^{10}\)Another interesting choice of \( c \) in Eq. (11) is \(-1\). Then each term in this expansion is positive definite and the series monotonically converges to the exact value. To any given order \( n \) of the expansion, one obtains a lower bound to the exact energy. However, the convergence is not as fast as the choice of \( c = \langle \tilde{T} \rangle \).


