Midgap transition of domain walls in superconductors

2000 J. Phys.: Condens. Matter 12 L147

(http://iopscience.iop.org/0953-8984/12/7/102)

J. Phys.: Condens. Matter **12** (2000) L147–L153. Printed in the UK PII: S0953-8984(00)08821-4

LETTER TO THE EDITOR

Midgap transition of domain walls in superconductors

S M M Virtanen and M M Salomaa

Materials Physics Laboratory, Helsinki University of Technology, PO Box 2200 (Technical Physics), FIN-02015 HUT, Finland

Received 19 October 1999

Abstract. The electronic structure of domain walls in superconductors is computed as a function of temperature within Bogoliubov–de Gennes theory. We find a spontaneous interface transition at an ultralow temperature $T_\star \approx 10^{-2}T_c$, in which the self-consistent pair potential transforms from a smooth Ginzburg–Landau form into one showing oscillatory Friedel-like behaviour. The transition is associated with a lifting of the energy of midgap excitations and the formation of an energy minigap. Like the bulk superconducting phase transition at T_c, this midgap transition is manifested as a pronounced peak in the specific heat of the domain-wall matter. The transition is also predicted to occur in thin SNS (superconducting–normal–superconducting) Josephson π-junctions.

Domain walls are planar interfaces between distinct degenerate ground states, or vacua, of bulk matter. Physical systems with a spontaneously broken discrete symmetry may be expected to exhibit such structures. These planar objects span across regions of space, 'false vacua', where the order parameter in the condensed medium is locally inhomogeneous, interpolating between the distinct asymptotic ground states [1]. Particularly interesting domain-wall structures have been predicted to occur in superfluid ^{3}He, in which the A- and B-phase domain walls [2] display superfluid core structures that carry spontaneous spin and/or mass supercurrents along the interface, thus providing laboratory models for cosmic domain walls [3].

Due to the inhomogeneity of the order-parameter distribution, domain walls can confine excitations. Recently, Hu [4] predicted that a sizable areal density of surface states at the Fermi energy, or midgap states, would occur as a novel signature for d-wave pairing in superconductors. In contrast to the usual exponential behaviour of the specific heat for s-wave pairing, such midgap states give rise to a power-law temperature dependence. Therefore, the occurrence of midgap states and the behaviour of the specific heat have been proposed as indicators distinguishing between s- and d-wave pairing, in particular for high-temperature superconducting materials.

Experimentally, in addition to the specific heat measurements, zero-bias conductance peaks in proximity-electron-tunnelling spectroscopy [5–7] have been used as an indicator for midgap states. The electronic structure and thermodynamic properties of domain walls in superconductors have been discussed by a number of authors, mostly within the Andreev approximation and/or quasiclassical theory [8–12]. The energies of surface midgap states have also been investigated: in most cases, they have been found to equal zero, except under special circumstances, such as when the order parameter possesses mixed symmetry or the surfaces are rough [13–16]. On the other hand, in the self-consistent microscopic calculations reported thus far [17–23], the thermodynamical aspects of such structures have not been addressed.

Here we report calculations carried out within the Bogoliubov–de Gennes (BdG) formalism [24, 25] to investigate the thermodynamics of a domain-wall structure exhibiting midgap states. The results show interesting and novel features which only arise when the superconducting excitation spectrum and the pair potential are computed fully self-consistently. We find that, for decreasing temperature, the electronic spectrum undergoes a spontaneous transition at $T_\star \approx 10^{-2}T_c$. Due to admixture, the midgap states are simultaneously lifted to form an energy minigap and the superconducting pair potential develops strong Friedel oscillations in the vicinity of the domain wall. This restructuring of the domain-wall matter is found to be associated with a characteristic peak in the specific heat.

The occurrence of midgap surface states in superconductors is related to the antisymmetry of the order parameter in momentum space or in the real space. In this letter, we investigate BdG equations for an antisymmetric domain wall, in vanishing external magnetic field. We search for self-consistent solutions of pair potentials in the form $\Delta(-x) = -\Delta(x)$. An SNS Josephson junction with a large cross-sectional area (compared to the thickness of the junction) and a phase difference $\Delta\varphi = \pi$ between the superconducting electrodes is an example of such a domain wall. In the following, we focus on the limit where the thickness d of the normal layer tends to zero; however, our computations show that the results also hold, qualitatively, for Josephson junctions with d of the order of the coherence length. Moreover, here we only consider conventional s-wave pairing.

Due to the translational invariance in the y- and z-directions, the quasiparticle amplitudes may be expressed as

$$\psi(\boldsymbol{r}) = \begin{pmatrix} u(\boldsymbol{r}) \\ v(\boldsymbol{r}) \end{pmatrix} = \mathrm{e}^{\mathrm{i}\xi_0(k_y y + k_z z)}\phi(x). \tag{1}$$

We measure lengths in units of the zero-temperature coherence length $\xi_0 \equiv \hbar v_\mathrm{F}/\Delta_0$ (v_F is the Fermi velocity and Δ_0 the bulk gap at $T = 0$), and energies in units of Δ_0. This yields BdG equations in the form

$$\sigma_z\left[-\frac{1}{2k_\mathrm{F}\xi_0}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - E_\mathrm{F}^\perp\right]\phi(x) + \sigma_x\Delta(x)\phi(x) = E\phi(x) \tag{2}$$

where σ_x, σ_z denote Pauli matrices, k_F is the Fermi wavenumber, and

$$E_\mathrm{F}^\perp \equiv E_\mathrm{F} - \frac{\xi_0}{2k_\mathrm{F}}(k_y^2 + k_z^2) \tag{3}$$

where E_F is the Fermi energy. The pair potential is determined from the implicit self-consistency condition

$$\Delta(\boldsymbol{r}, T) = g\sum_i u_i(\boldsymbol{r})v_i^*(\boldsymbol{r})[1 - 2f_i(T)]. \tag{4}$$

Here g is the effective electron–electron coupling constant and f the Fermi function. The sum includes all positive energy eigensolutions of equation (2) below the Debye cut-off $E_\mathrm{D} \equiv \hbar\omega_\mathrm{D}/\Delta_0$. It is to be noted that, owing to symmetry, the supercurrent density vanishes, thus confirming the consistency of setting the magnetic field equal to zero.

We search for self-consistent solutions of the BdG equations iteratively: at each iteration step a new pair potential is computed from equation (4), using the quasiparticle solutions corresponding to the current pairing amplitude, until convergence. The equations are solved in a semi-infinite slab $|x| \leqslant L$ with $L \gg 1$, imposing Dirichlet boundary conditions for the quasiparticle amplitudes at $x = \pm L$. Antisymmetry of the pair potential is utilized to halve the computational domain to the interval $0 \leqslant x \leqslant L$. As in reference [18], we use a finite-difference discretization method to cast equation (2) into the form of an eigenvalue problem with a narrow-banded coefficient matrix. Finally, the eigensolutions are computed using the Lanczos method implemented in the ARPACK library routines. When the number of eigensolutions required is moderate, this turns out to be an efficient and, in particular, easily implementable way to solve the BdG equations.

In the computations presented here we used the dimensionless Fermi energy $E_F = 34$, and took $k_F\xi_0 = 68$. The cut-off energy was $E_D = 2.7$ (the parameter values correspond to those used in [26] to model $NbSe_2$, a layered type II material), and the width of the slab $2L = 12$ which is large enough for finite-size effects to be negligible. Moreover, we performed extensive computations varying the parameter values over wide ranges, and in addition considered a cylindrical Fermi surface by neglecting the k_z-dependence in equation (3).

Results of our calculations are presented in figures 1 to 4. We computed the self-consistent electronic structure of the domain wall at reduced temperatures T/T_c between 0.0001 and 1.3 at 250 points. To determine the specific heat, a high accuracy in the self-consistency is essential: the iteration process was repeated until the relative difference between the pair potentials at successive steps decreased to less than 10^{-5}. The quasiparticle states below the cut-off E_D lie in the interval $E_F^{\perp} \in [-E_D, E_F]$, which we discretized with an equally spaced grid

$$(E_F^{\perp})_j = (1 - s_j)(-E_D) + s_j E_F \qquad s_j = \left(j - \frac{1}{2}\right)\Big/ N. \tag{5}$$

The density of states for a closed Fermi surface is constant with respect to the parameter s. The number of grid points is dictated by the desired accuracy; we used $N = 1000$.

The energy spectrum of quasiparticle excitations at the temperature $T = 10^{-3}T_c$ is displayed in figure 1. Above the gap edge, it features a dense contribution from the scattering states; below it, there are a few bound-state branches of localized quasiparticles. The lowest branch—midgap states—is almost dispersionless for $s < 0.9$, and has a very small but finite average energy. The existence of such a midgap branch is characteristic for antisymmetric pair potentials [4, 15].

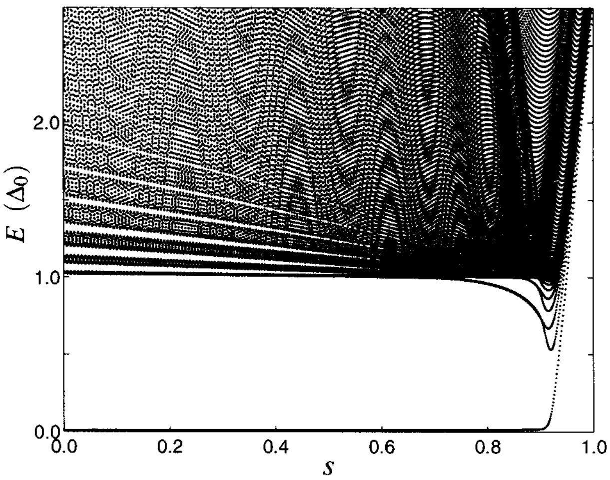

Figure 1. A self-consistent energy spectrum at $T = 10^{-3}T_c$ for quasiparticle excitations within an antisymmetric domain wall as a function of the parameter s; this parameter, describing the quasiparticle momentum in the plane of the domain wall, is defined in equation (5). Note, in particular, the lowest branch—midgap excitations—for energies $E_{mid} \ll \Delta_0$.

The self-consistent pair potential in the vicinity of the domain wall is presented in figure 2 as a function of temperature. At $T_\star \approx 10^{-2}T_c$, the pair amplitude exhibits an abrupt transition between Ginzburg–Landau behaviour and an ultralow-temperature form with strong Friedel

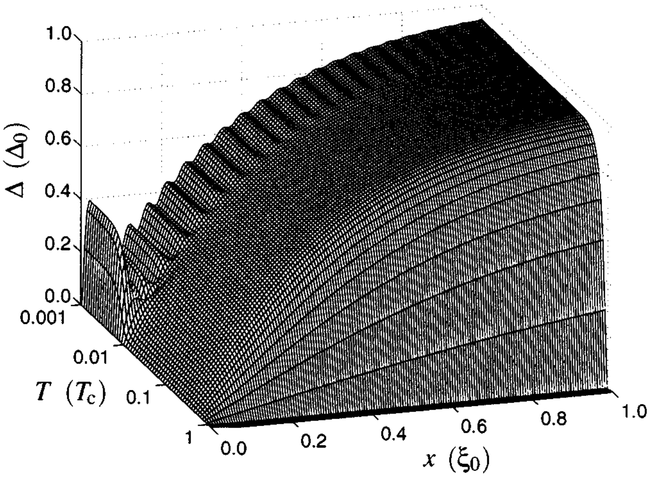

Figure 2. The self-consistent superconducting pair potential $\Delta(x, T)$ in the domain-wall region as a function of temperature (T, logarithmic scale). Note the Ginzburg–Landau shape for a wide temperature range below T_c and the transition into Friedel oscillations at $T_\star \approx 10^{-2}T_c$; the latter occur in the (x, T) region where the thermal excitations are quasinormal and localized.

oscillations—where the wavelength of the oscillations is π/k_F throughout the whole x-range, as expected for Friedel oscillations. This transition is associated with the crossing of the level indicating thermal energy (dashed line) and the midgap branch, as seen in figure 3. At temperatures above $T_\star$, the lowest-energy states in the midgap branch are within numerical accuracy zero-energy excitations ($E \lesssim 10^{-5}\Delta_0$) and the pair potential rises monotonically to its asymptotic value. In the transition, this bound-state branch is lifted to a finite energy and an energy minigap of order $E \sim k_B T_\star$ is developed. Simultaneously, the Friedel oscillations appear in the pair potential. In the region $T \lesssim T_\star/2$, the temperature dependence is saturated.

The Friedel oscillations are generated entirely by the states in the midgap branch. This is illustrated in the lhs series of figure 3, where the contribution of the other states to the pair potential (cf. equation (4)) is represented by dashed lines. Due to the domain wall, the localized midgap states are phase coherent, so their oscillatory contributions to the pair potential add constructively to produce strong Friedel oscillations. Because of hybridization [15], these oscillations break the particle–hole symmetry of the zero-energy states, and lift the midgap branch states to small but nonzero energies. When the temperature is increased such that the thermal energy corresponds to the energies of the uplifted midgap states, their contributions to the pair potential, and hence the Friedel oscillations, are suppressed. This weakens the hybridization effect, lowering the energies of the midgap states even further. For temperatures above $T_\star$, the oscillations disappear and the midgap states tend towards zero energy.

This interface transition would be reflected in the scanning tunnelling microscopy spectrum [27, 28] for domain walls. Also, the resonant absorption of microwave power [29] could be used to measure the energy shift of the midgap states. The transition closely resembles the second-order phase transition at T_c, in which the pair potential develops and the gap edge crosses the thermal energy (however, this analogy is not exact owing to the strong dispersion of the midgap state branch at $0.9 < s < 1.0$). Figure 4 displays the computed specific heat density of the Fermi quasiparticle excitations. Like the transition at T_c, the midgap transition is associated with a peak in the specific heat (the relative heights of the peaks at $T_\star$ and T_c depend on the width of the slab since the midgap transition takes place only in the vicinity

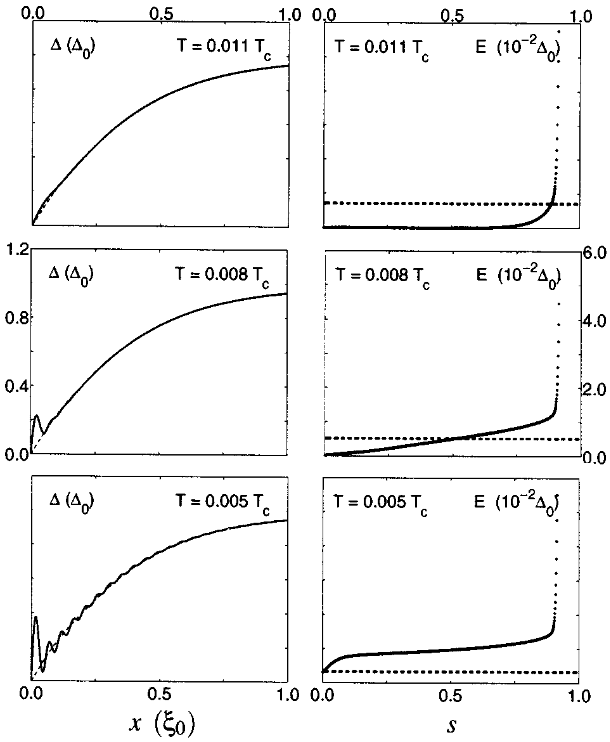

Figure 3. The transition, in detail, of the pairing amplitude (lhs) from the smooth GL form into that of the Friedel phase. The rhs illustrates the simultaneous lifting of the zero-energy midgap branch to the finite minigap energy $E_{\rm mid} \sim k_{\rm B}T_{\star}$. At the transition, the midgap branch crosses the thermal energy (dashed level). The dashed lines on the lhs represent contributions of the states above the midgap branch ($E \geqslant 0.02\Delta_0$) to the pair potential.

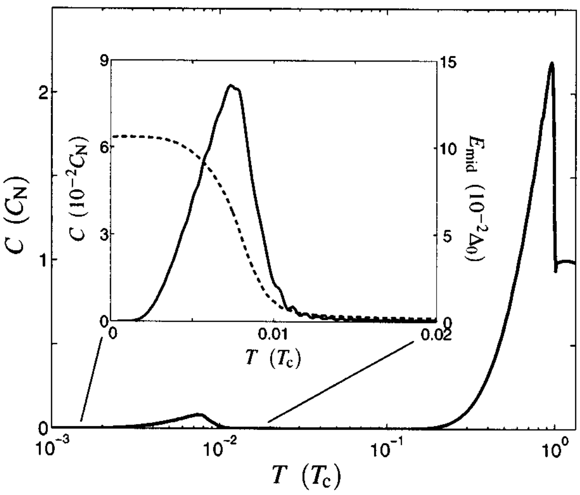

Figure 4. Normalized specific heat $C/C_{\rm N}$ ($C_{\rm N}$ denotes the specific heat in the normal state at $T_{\rm c}$) of the domain wall as a function of temperature. The inset shows the domain-wall transition region, where the specific heat (continuous curve) exhibits a pronounced peak. The dashed line represents the averaged energy of the midgap states with $E \leqslant 0.02\Delta_0$.

of the domain wall. Qualitatively, our results hold for a wide range of parameter values. However, the topology of the Fermi surface affects also the qualitative features of the interface transition by modifying the dispersion of the midgap states. For an open cylindrical Fermi surface, the transition is even sharper, but it manifests itself in a doubly peaked structure of the specific heat). The thermodynamics of inhomogeneities in BCS superconductors at temperatures $T \ll T_c$ is determined by the midgap states, provided that they exist. Nontrivial structure in the thermodynamic quantities at ultralow temperatures is an indication for the existence of midgap excitations.

The results displayed correspond to an SNS Josephson π-junction in the limit where the thickness d of the normal layer approaches zero. Since this limit is energetically unstable, we have also modelled finite-width π-junctions by allowing the effective coupling constant g to have spatial dependence, smoothly vanishing in the region $|x| < d/2$. Our computations show that the midgap transition is a fairly robust phenomenon: the essential qualitative features of the transition remain for $k_F^{-1} \sim d < \xi$. The Josephson effect is at low temperatures dominated by the low-energy midgap excitations; see [30]. Therefore, the midgap transition should manifest itself as a low-temperature Josephson anomaly in which the excitations suddenly acquire an energy minigap. Thus we expect these phenomena to be observable in physically realizable thin Josephson π-junctions.

In conclusion, we have computed the temperature dependence of the electronic structure for an antisymmetric domain wall (modelling, e.g., a thin Josephson π-junction) in a superconductor, using the Bogoliubov–de Gennes theory. We have found a novel transition at temperatures corresponding to the energy of midgap states, in which the pair potential develops strong Friedel oscillations in the vicinity of the domain wall, and the midgap excitation branch is lifted to a finite energy. This transition has features similar to the second-order bulk phase transition at T_c; in particular, it is associated with a pronounced peak in the specific heat.

The Academy of Finland is acknowledged for support of SMMV within the Graduate School in Technical Physics; the Centre for Scientific Computing (CSC, Finland) is thanked for computer resources.

References

[1] Wilets L 1989 *Nontopological Solitons* (Singapore: World Scientific)
[2] Salomaa M M and Volovik G E 1988 *Phys. Rev.* B **37** 9298
Salomaa M M and Volovik G E 1989 *J. Low Temp. Phys.* **74** 319
[3] Vilenkin A and Shellard E P S 1994 *Cosmic Strings and other Topological Defects* (Cambridge: Cambridge University Press)
[4] Hu C-R 1994 *Phys. Rev. Lett.* **72** 1526
[5] Kashiwaya S, Tanaka Y, Koyanagi M, Takashima H and Kajimura K 1995 *Phys. Rev.* B **51** 1350
[6] Tanaka Y and Kashiwaya S 1995 *Phys. Rev. Lett.* **74** 3451
[7] Alff L, Takashima H, Kashiwaya S, Terada N, Ihara H, Tanaka Y, Koyanagi M and Kajimura K 1997 *Phys. Rev.* B **55** R14 757
[8] Bar-Sagi J and Kuper C G 1972 *Phys. Rev. Lett.* **28** 1556
Bar-Sagi J and Kuper C G 1974 *J. Low Temp. Phys.* **16** 73
[9] Buchholtz L J, Palumbo M, Rainer D and Sauls J A 1995 *J. Low Temp. Phys.* **101** 1079
Buchholtz L J, Palumbo M, Rainer D and Sauls J A 1995 *J. Low Temp. Phys.* **101** 1099
[10] Matsumoto M and Shiba H 1995 *J. Phys. Soc. Japan* **64** 3384
Matsumoto M and Shiba H 1995 *J. Phys. Soc. Japan* **64** 4867
Matsumoto M and Shiba H 1996 *J. Phys. Soc. Japan* **65** 2194
[11] Xu J H, Miller J H Jr. and Ting C S 1996 *Phys. Rev.* B **53** 3604
[12] Barash Yu S, Svidzinsky A A and Burkhardt H 1997 *Phys. Rev.* B **55** 15 282
[13] Yang J and Hu C-R 1994 *Phys. Rev.* B **50** 16 766

[14] Nagato Y and Nagai K 1995 *Phys. Rev.* B **51** 16 254
[15] Ohashi Y and Takada S 1996 *J. Phys. Soc. Japan* **65** 246
[16] Walker M B, Pairor P and Zhitomirsky M E 1997 *Phys. Rev.* B **56** 9015
[17] Stojković B P and Valls O T 1993 *Phys. Rev.* B **47** 5922
[18] Troy R J and Dorsey A T 1995 *Phys. Rev.* B **51** 11 728
[19] Šipr O and Györffy B L 1995 *J. Phys.: Condens. Matter* **7** 5239
Šipr O and Györffy B L 1996 *J. Phys.: Condens. Matter* **8** 169
[20] Feder D L, Beardsall A, Berlinsky A J and Kallin C 1997 *Phys. Rev.* B **56** R5751
[21] Yan X-Z and Iyetomi H 1998 *Phys. Rev.* B **57** 7944
[22] Martin A M and Annett J F 1998 *Phys. Rev.* B **57** 8709
[23] Zhu J-X, Friedman B and Ting C S 1999 *Phys. Rev.* B **59** 3353
[24] de Gennes P G 1989 *Superconductivity of Metals and Alloys* (New York: Addison-Wesley)
[25] Ketterson J B and Song S N 1999 *Superconductivity* (Cambridge: Cambridge University Press)
[26] Gygi F and Schlüter M 1991 *Phys. Rev.* B **43** 7609
[27] Levi Y, Millo O, Rizzo N D, Prober D E and Motowidlo L R 1998 *Phys. Rev.* B **58** 15 128
[28] Virtanen S M M and Salomaa M M 1999 *Phys. Rev.* B **60** 14 581
[29] Aberle H and Kümmel R 1986 *Phys. Rev. Lett.* **57** 3206
[30] Yan X-Z and Hu C-R 1999 *Phys. Rev. Lett.* **83** 1656