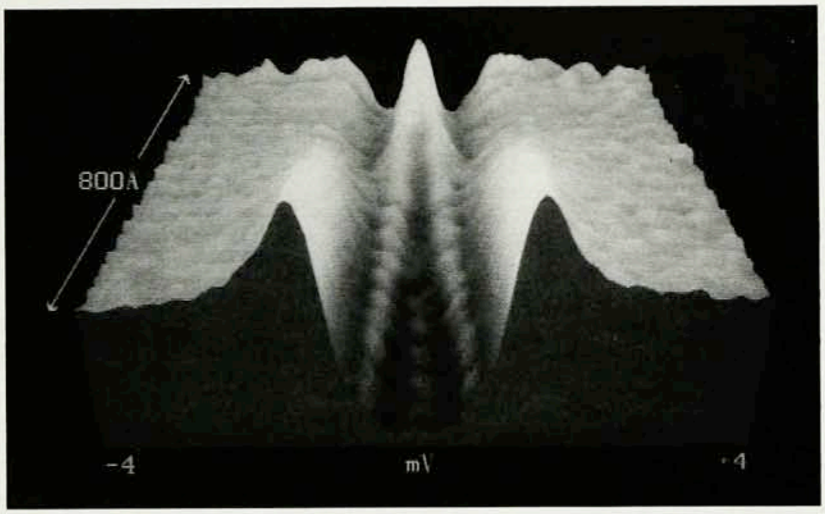
STM UNRAVELS THE VORTEX CORE IN TYPE II SUPERCONDUCTORS

When two conductors are brought so close together that wavefunctions of electrons in them begin to overlap appreciably, electrons in one of the conductors may tunnel into the other. The magnitude of this tunneling current depends, if the current flows, say, from a probe tip to a surface to be probed, primarily on the probability that electron states having energy and momentum similar to those of electrons in the tip exist and are unoccupied in the surface to be probed. The scanning tunneling microscope, in which a metal probe scans a surface and the tunneling current at various positions is measured, therefore yields information about the nature and density of electron states on the scanned surface. STM studies of a clean surface of 2H-$NbSe_2$ when it is superconducting have now revealed new and unexpected features in the spectrum of electron states in magnetic flux lines in superconductors. The remarkable spatial resolution of the STM, which has steadily yielded new and interesting results about physics at surfaces since the instrument was invented, once again underlies the new discoveries: Without the STM it might not have been possible to probe electronic states on the scale of a few angstroms.



Two ridges begin to appear at a distance of several coherence lengths from the vortex core in the tunneling conductance between the STM tip and the 2H-$NbSe_2$ surface, confirming a theoretical prediction that arose out of attempts to understand the peak, observed last year, in the density of states at the center of a vortex core. The separation between the ridges decreases with decreasing distance from the core until they merge at the core center into the peak observed last year. This perspective view was obtained by measuring the tunneling conductance at 128 points along a line normal to the flux filament and going through the vortex core. Both the tip and the surface were kept at 0.3 K and a magnetic field of 500 gauss acted on the superconductor. The coherence length under these conditions is about 77 Å. The front end of the image is at a distance of 600 Å from the core center. (Courtesy Harald Hess.)

Electrons are paired in the ground state of a superconductor, so it costs energy to break a pair and create an excitation having energy–momentum dispersion similar to that of an almost freely propagating particle: One says that the spectrum of one-particle excitations in a superconductor has a gap. In a normal metal, by contrast, single particles may be excited across the Fermi surface at almost no energy cost if the particle momentum is close to the Fermi momentum. (Single-particle excitations are also called quasiparticle excitations.)

The tunneling current, which the STM measures with remarkable spatial resolution, also depends on the separation between the tip and the scanned surface. In many applications using the STM, the height of the tip above the surface is adjusted for constant magnitude of the tunneling current. The recent study of the electronic structure of a vortex core, by contrast, measured the change in the tunneling current per unit change in the bias voltage applied between the tip and the surface held at a fixed separation. The differential conductance is a probe, as hinted earlier, of the density of states for single-particle excitations per unit energy of those excitations. This measure of the energy spectrum also is different in a superconductor from that in a normal metal. In a normal metal it is almost constant for energies close to the Fermi energy; in a superconductor it is zero for energies (measured with respect to the Fermi energy) less than the gap energy, rises abruptly at the gap energy to a value larger than the value in the normal state and settles to the normal-state value at larger energies.

Local gap function

The behavior discussed above for the density of single-particle excitations in a superconductor is valid at each point in a type I superconductor. (A type I superconductor is a perfect diamagnet in magnetic fields weaker than a critical value, but this superconducting phase is destroyed in fields stronger than the critical value.) The unprecedented spatial resolution of the STM is therefore not needed to obtain the density of states in a superconductor; the density of states can be obtained simply by measuring the tunneling conductance of a junction formed by a metal and a superconductor separated by a thin layer of an insulator. In 1960, Ivar Giaever (then at the General Electric Research and Development Center in Schenectady) measured the tunneling conductances of junctions formed by lead and aluminum and by lead and magnesium at temperatures at which one of the metals (lead) was a superconductor. His results confirmed the existence of the hole in the density of states around the Fermi energy.

The density of states in type II superconductors, such as the 2H-$NbSe_2$ that was recently studied using the STM, is more complex, however. As Alexei A. Abrikosov, who coined the term "type II superconductor," showed in 1957, a type II superconductor is a perfect diamagnet and behaves like a type I superconductor only when it is placed in a magnetic field weaker than a critical value called the lower critical field. Abrikosov also showed that for fields stronger than the lower critical value but weaker than another critical value called the upper critical field, at which superconductivity is destroyed and the whole sample becomes normal, magnetic flux exists in a type II superconductor in the form of filaments parallel to the direction of the applied field. In this so-called mixed state of a type II superconductor placed in a magnetic field, the magnetic field is maximum at the axes of the cylindrical filaments and decreases with radial distance at a rate given by a parameter called the field penetration depth. The flux filaments are also called vortex lines, because the supercurrent that flows around them has a nonzero curl and the dependence of the supercurrent on the radial distance from the axes is similar to that of the velocity field around a vortex in fluid flow. The existence of vortex lines and their arrangement in a periodic array called the Abrikosov lattice—a triangular lattice formed by the points at which the lines intersect a plane normal to them—have been confirmed in a variety of experiments. The experiments include observation of Bragg scattering in the elastic scattering of neutrons from the periodic Abrikosov lattice; comparison of the position and shape of an nmr line in the superconducting state with that in the normal state; and magnetic decoration, in which a surface of the superconductor normal to the flux lines is exposed to a fine dust of magnetic particles and the particles settle preferentially in regions where the flux lines intersect the surface.

Like others of a large class of ordered phases, the superconductor is distinguished from the normal metal by the nonzero value of an order parameter. The superconductivity order parameter, also called the gap function, is a measure of the amplitude for electron pairing, and in simple situations its value may be related to that of the energy gap in the spectrum of single-particle excitations. The Abrikosov solution shows that in the mixed state of a type II superconductor the value of the order parameter is not the same at every point: It is zero at the axis of a filament and rises, as one moves away from the axis, to a roughly constant value that depends on material parameters, temperature and the magnetic field strength. The increase in the gap function to its constant value occurs over a distance called the coherence length. Type II superconductivity occurs when the energy of a surface separating superconducting and normal domains is negative, which is possible when the penetration depth is longer than $\sqrt{2}$ times the coherence length.

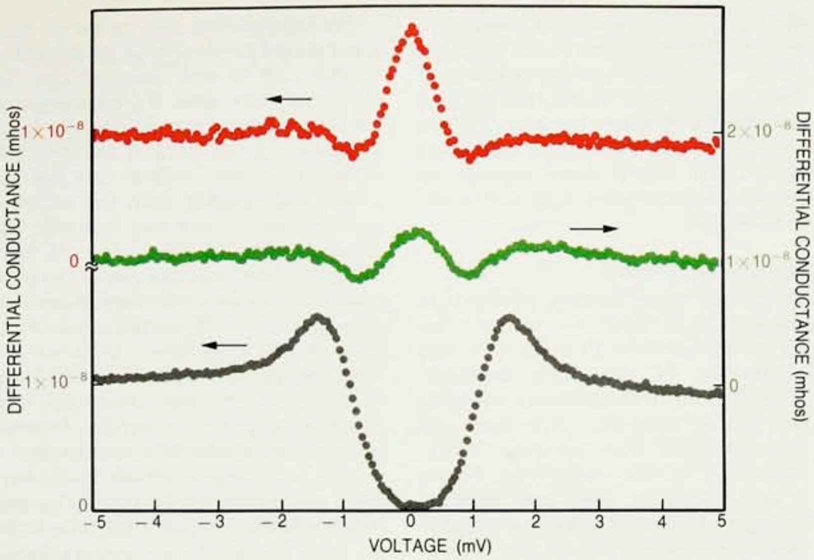
The spatially periodic behavior of the gap function in the mixed state implies that the density of single-particle excitations will be a periodic function of position in this state of a type II superconductor. The recent STM studies confirmed this simple expectation, but they also brought out an unexpected feature in the detailed form of the density of state at the center of the vortex core, namely, a peak at zero (Fermi) energy.

Zero-bias peak

Abrikosov obtained his solution for the vortex line in the context of the phenomenological equations for superconductivity that Vitaly Ginzburg and Lev Landau had proposed seven years earlier. Those equations are written in terms of the order parameter and therefore do not describe the spectrum or the density of single-particle excitations. In the microscopic BCS theory, however, both the spectrum and the wavefunctions of single-particle excitations may be obtained by solving the so-called Bogoliubov–de Gennes equations. (The Ginzburg–Landau equations may be derived from the microscopic BCS theory, as Lev Gorkov of the Landau Institute showed in 1959, two years after the theory was proposed. That theory therefore describes both the order parameter and the spectrum and density of single-particle excitations in the Abrikosov solution.)

Solving the Bogoliubov–de Gennes equations to obtain the spectrum of single-particle excitations near a flux line has drawn the attention of theorists intermittently since 1964, when Christiane Caroli, Pierre-Gilles de Gennes and Jean Matricon (all at Service de Physique des Solides, Orsay, at the time) made the first such attempt. Although an exact analytic solution has never been obtained, the approximate solutions suggested that the superconductivity gap would be reduced to a very small value in the vortex cores and that as far as the electron states with energies higher than the reduced-gap value were concerned, the flux filaments would act like normal metals for all practical purposes. The hole around the Fermi energy in the density of single-particle excitations, which, as pointed out above, is a characteristic of a superconductor or of a type II superconductor away from the vortex lines, would therefore get filled as one approached the vortex core. This was what one would have naively expected, Pierre Hohenberg (AT&T Bell Labs) explained to us, if one assumed that the density of states was a *local* function of the gap in the spectrum: Near the vortex core, where the Abrikosov solution said the order parameter would vanish, the density of states would have the form characteristic of a normal metal! Contrary to this expectation, however, studies last year by Harald F. Hess, Ralph B. Robinson, Robert C. Dynes, James M. Valles Jr and Joseph V. Waszczak (all at AT&T Bell Labs in Murray Hill) showed a prominent peak at the center of the energy gap when the STM scanned the vortex core.[1]

The figure on page 19 shows the tunneling conductance between a surface of 2H-$NbSe_2$ and the STM tip at 1.85 K as a function of the bias voltage between the tip and the surface for three different positions of the tip: 2000 Å away from the center of a vortex core, 75 Å from the center, and at the center. (The zero-field critical temperature for superconductivity in 2H-$NbSe_2$ is 7.2 K.) At 2000 Å away from the core center the voltage dependence of the conductance has the form sketched in almost all textbooks on superconductivity; the BCS theory predicts this form for tunneling between a superconductor and a normal metal, and Giaever first observed it in 1960. But as the tip scans towards the core center, the conductance at zero bias does not become flat in voltage, as would be expected if the density of states in the core had the form characterisitic of a normal metal and were flat in energy near the Fermi energy. Instead, the conductance develops a peak at zero bias. The zero-bias peak in the conductance implies that the density of quasiparticle states as a function of energy has a similar peak in the middle of the superconductive gap.



Tunneling conductance between the tip of an STM and a 2H-$NbSe_2$ surface measured when a magnetic field of 200 gauss acted on the surface and both the tip and the surface were kept at 1.85 K. Far away from a vortex core the conductance is zero for bias voltages less than the magnitude of the energy gap in one-particle excitations (gray, obtained when the tip was 2000 Å from the core center), but a peak in the middle of the gap appears when the tip scans the core. The green curve shows the conductance measured at a point 75 Å away from the center, and the red curve was obtained at the core center. It was expected before these measurements that near the core the conductance would be flat as a function of voltage. (Courtesy H. Hess.)

Theory predicts further structure

Observation of the zero-bias peak in the density of states at the vortex core came as a surprise to both theorists and experimenters. A simple, phenomenological theory that took away at least some of the surprise from the new observation was proposed by Albert Overhauser (Purdue University) and Luc L. Daemen (now at Los Alamos National Laboratory), who showed that the peak arose if one coupled the electrons in flux filaments, modeled as cylinders of normal metal with radii on the order of a coherence length, with the quasiparticle excitations of a superconductor.[2] But a microscopic understanding of the peak in the context of the Bogoliubov–de Gennes equations for single-particle excitations in the BCS theory became available only when those equations were solved numerically last year, soon after Overhauser and Daemen put forth their theory. The numerical solutions were obtained by Joel D. Shore, Ming Huang, Alan T. Dorsey and James P. Sethna (all at Cornell at the time) and by François Gygi and Michael Schlüter (AT&T Bell Labs).[3] Independently, Ulf Klein (Universität Linz) solved numerically equations describing a quasiclassical approximation to the microscopic theory of superconductivity and also obtained the zero-bias peak.[3]

The numerical solutions of the Bogoliubov–de Gennes equations available to date, as well as the earlier approximate, analytical solutions, are for a single flux tube in a superconducting background. The equations have both bound-state and scattering-state solutions. The angular momentum about the vortex core is among the quantum numbers characterizing the solutions. As expected for eigenfunctions in a cylindrically symmetric potential, the larger the angular momentum of a bound state is, the farther away from the axis the wavefunction has its maximum magnitude and the higher the energy of that bound state is.

The recent solutions of the Bogoliubov–de Gennes equations show that the mid-gap peak at the vortex center arises from low-angular-momentum bound states, whose wavefunctions are maximum near the vortex center. At zero bias, these wavefunctions have the largest overlap with those of electrons in the tip when the tip is centered on the vortex center.

Already in 1964 Caroli, de Gennes and Matricon knew that the Bogoliubov–de Gennes equations have bound-state solutions near a vortex core. Could they have discovered the position dependence of the density of states in a core? It is only since the invention of the STM that electronic properties can be probed locally on length scales on the order of a few angstroms. One might therefore say, retrospectively, that the reason theorists did not discover the peak is that nobody thought it meaningful or experimentally significant to discuss the *local* density of states on a length scale much shorter than a coherence length. After the STM found the peak, however, the Cornell group predicted a new feature in the density of states away from the core center—namely, a double peak. Wavefunctions that have maximum amplitude at some distance from the core center have energies that are symmetric about the Fermi energy (center of the gap). These wavefunctions should cause a pair of symmetric maxima in the differential conductance as a function of the bias voltage.

This prediction motivated the Bell Labs group to repeat the experiment at a lower temperature and thereby improve the voltage (or energy) resolution. The figure on page 17 shows a perspective plot of the tunneling conductance between a surface of 2H-$NbSe_2$ and the STM tip at 0.3 K. The perspective was obtained by measuring the tunneling conductance at 128 points along a line going through the vortex core. At each point the conductance was measured for several values of the bias voltage between the tip and the surface. The front end of the perspective view, at a distance of 600 Å from the core, shows the characteristic superconductive hole around zero bias voltage. But two ridges develop in the gap as one approaches the core center. The separation (in bias voltage) between the ridges decreases, and their amplitude increases, with decreasing distance from the center, so that very near the center they merge into the one big peak observed earlier.[4]

In their solution, Gygi and Schluter studied both bound and scattering states. The scattering states are important for the bias dependence of the conductance away from the superconductivity hole, that is, for bias values at which the conductance rises from zero and then settles to its constant value. The self-consistent solution of Gygi and Schlüter shows that not just the density of states but also the gap function may show fine structure; that is, it might have ripples on length scales smaller than the coherence length.

Sixfold symmetry

There are three further effects that theories must take into account: interaction between flux lines or the possibility of tunneling between states bound to neighboring vortices; the role of material impurities and imperfections; and the role of the symmetry of the underlying $NbSe_2$ crystal structure. Gygi and Schlüter and, independently, Klein have examined the modifications in the tunneling conductance due to interaction between flux lines. Klein also reports that the height and width of the zero-bias peak depends on parameters measuring impurities and imperfections in the materials.[5]

The picture on the cover of this issue shows the conductance around a vortex core at zero bias voltage. In the color code used, the conductance (or the density of states) is larger than the value in the normal state of 2H-$NbSe_2$ in white, yellow and red regions, and smaller than the normal-state value in green and blue regions. Similar plots of data at fixed bias voltages show that the size of the core region increases with increasing magnitude of the bias voltage, indicating that the STM probes wavefunctions that are increasingly spread out from the center. The plots also show six-fold symmetry in the angular dependence of the density of states around a vortex, which arises from the hexagonal symmetry of the $NbSe_2$ lattice. The six-fold pattern undergoes a twist at some value of the bias voltage.[4] Schlüter told us that the energy spectrum, when regarded as a function of, or as having a "band structure" in, angular momentum, splits into two branches (or sub-bands) when the Bogoliubov–de Gennes equations are coupled to the underlying lattice. The branch of the spectrum that the STM tip probes changes at some value of the bias voltage, causing the twist because the sub-bands have different symmetry orientations.[6]

Earlier attempts to use the STM to study the density of states in type II superconductors probably suffered from poor surface quality, Hess conjectures. —ANIL KHURANA

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GIGANTIC STRUCTURES CHALLENGE STANDARD VIEW OF COSMIC EVOLUTION

These are exciting times for cosmologists. The "standard cosmological model" that purports to describe the evolution of the universe is being tested at both ends by spectacular astronomical observations. On the one hand are the recently discovered "Great Wall"[1] and "Great Attractor,"[2] enormous agglomerations of galaxies that attest to coherent structures stretching over half a billion light years in the present epoch. On the other hand are the new measurements of the uniformity of the cosmic microwave background, which tell us that the universe was amazingly smooth when it first became transparent—some 300 000 years after the Big Bang. The question at issue is: How did the cosmos evolve from these almost wrinkle-free beginnings to a present-day structure of such manifest inhomogeneity?

The standard hot Big Bang model, first formulated by George Gamow in the 1940s, nowadays generally incorporates the hypotheses of inflation and cold dark matter. It presumes that the density perturbations which eventually gave rise to galaxy clusters began as quantum fluctuations that were enormously stretched during the inflationary expansion phase in the first 10^{-35} sec after the Big Bang. After the universe was rendered transparent by the decoupling of radiation and matter, the standard model asserts, all further clustering of matter was due entirely to the ponderous action of gravity working against the general Hubble expansion.

The inflationary scenario (see PHYSICS TODAY, September 1987, page 61) requires that the mean mass density of the universe be very close to its "closure" value—about 100 times the mass that can be accounted for by luminous stars. In the standard model, most of the remaining, *dark* matter is presumed to consist of weakly interacting particles whose thermal velocities would have been negligible in the epoch when structure started to develop. Hence the adjective "cold," which serves to distinguish this model from those that attribute most of the dark mass to neutrino-like particles, whose relativistic thermal motion would tend to wipe out density fluctuations.

Problems

When it was first developed in the early 1980s, inflationary cosmology was prized as the only theory that offered a causal mechanism for the origin of perturbations large enough to account for the creation and clustering of galaxies. That is to say, inflation guarantees that all the universe observable today would have grown from a primordial region small enough to be encompassed within the causal horizon defined by the speed of light. In fact, inflation is the only theory whose predictions—in particular, its initial spectrum of density perturbations—are sufficiently detailed to permit a serious confrontation with the data.

As the decade and its observing technology progressed, extensive redshift surveys accumulated more and more evidence that galaxies were clustering into structures much larger than anything the inflation theortists were expecting. Even when helped along by cold dark matter and the *ansatz* of "biased galaxy formation," computer simulations of gravitational evolution starting from the spectrum of density fluctuations left behind by inflation were unable to generate structures much larger than 30 Mpc. (A megaparsec is slighty more than 3 million light-years. All distances quoted here take the Hubble constant H_0 to be 100 km/sec per Mpc. If H_0 turns out to be smaller, all distances inferred from redshifts become correspondingly larger.)

The Great Wall, the most extended of the recently discovered megastructures, appears to stretch over 170 Mpc. In their attempts to understand