



Superconducting Characterization Tools and Techniques (Part II)

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Outline

- Density of States
- Superconducting Gap Equation
- Electron Tunneling
- Application: planar tunnel junction
- Principle of STM/STS
- **STM** and Superconductors
- □ Vortices in Type II Superconductors
- **STM** application to Superconducting Qubits



Density of States of Metals

For free electrons:

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

The density of states, i.e. the number of available states between ε and $\varepsilon + d\varepsilon$ is:



□ Very important result, but note that the E dependence is different for different dimension (1D, 2D, 3D).

- $\Box \text{ Normally } k_B T \ll \varepsilon_F \text{ even at room T}$
- □ For most metals $N(\varepsilon_F) \approx constant$
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Key-ideas of the BCS theory of 1957 (**Bardeen, Cooper, Schrieffer**)

- □ The interaction of the electrons with lattice vibrations (phonons) must be important (isotope effect, high transition temperature for some metals which are poor conductors at room temperature).
- □ The electronic ground state of a metal at 0 K is unstable if one permits a net attractive interaction between the electrons, no matter how small.
- □ The electron-phonon interaction leads to a new ground state of Bosonic electron pairs (Cooper pairs) which shows all the desired properties.



BCS: Microscopic Theory of Superconductivity



1957: Bardeen, Cooper, Schrieffer Nobel:1972

PHYSICAL REVIEW



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DECEMBER 1, 1957

Theory of Superconductivity*

J. BARDEEN, L. N. COOPER,[†] AND J. R. SCHRIEFFER[‡] Department of Physics, University of Illinois, Urbana, Illinois (Received July 8, 1957)

Electron has charge -e

$$| \rightarrow \neg \mathcal{V} \mathcal{V} \mathcal{V} \rightarrow |$$

Scattering of electrons produces resistance.

A <u>current</u> generates a <u>voltage</u>, and hence cause dissipation

Electrons are paired together: Cooper pairs have charge -2e



Cooper pairs carry a supercurrent, which encounters no resistance

A supercurrent generates no <u>voltage</u>, and hence cause no dissipation



Superconductors: Gap Equation

NORMAL METAL:
$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

SUPERCONDUCTOR: $E = \sqrt{\varepsilon_k^2 + \Delta^2}$



SUPERCONDUCTING QUASIPARTICLE DENSITY OF STATES:

$$N_{S}(E) = N_{N}(E_{F}) \frac{|E|}{\sqrt{E^{2} - \Delta^{2}}}$$



Microscopic theory of superconductivity: Bardeen, Cooper, Schrieffer (BCS) 1957



- □ In a normal metal, electrons obey the Fermi statistics and the Pauli exclusion principle
- □ In a superconductor, electrons are paired in Cooper Pairs. They all condense in the ground state. An energy gap D opens above the Fermi energy.





Electron Tunneling



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Electron tunneling through a potential barrier



In quantum mechanics a particle can penetrate into a barrier where it would be classically forbidden.



Electron tunneling through a potential barrier

What is the probability that an incident particle tunnels through the barrier?



Time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(z)\right)\psi(x) = E\psi(x)$$

Getting an exact result requires applying the boundary conditions at x=0 and x=L

Free electron solutions in region I and III

Exponential decay in the barrier (region II)

The electron tunnels through the barrier.

$$\psi_{I} = e^{ikx} + Ae^{-ikx}$$
$$\psi_{III} = De^{ikx}$$

$$\psi_{II} = Be^{-Kx} + Ce^{Kx}$$

 $k^{2} = 2mE/\hbar^{2}$ $K^{2} = 2m(U_{0} - E)/\hbar^{2}$ $M = S^{2} M =$

Electron tunneling through a potential barrier



What is the probability that an incident particle tunnels through the barrier?

In many situations, the barrier width L is much larger that the "decay length" 1/K of the penetrating wave ($KL \ll 1$). In this case $C \approx 0$.

Transmission coefficient: transmitted/incoming amplitudes

T
$$\approx Ge^{-2KL}$$
 where $G = 16\frac{E}{U_0}\left(1-\frac{E}{U_0}\right) = 16\frac{2m}{\hbar^2}\frac{k^2K^2}{k^2+K^2}$

T decays exponentially with the barrier width.



Application: planar tunnel junction





Tunneling electrons obey Fermi statistics:

$$f(E) = \frac{1}{\rho^{E/k_B T + 1}} \qquad \qquad E = \mathcal{E} - \mathcal{E}_F$$



Tunneling depends on the electronic density of states (DOS) of both electrodes in the junction.



Planar Tunnel Junctions



T(E,V)is the transmission factor, N_L and N_R are the density of states in the two electrodesf(E)is the Fermi function, which guaranties that the electrons tunnel from an occupied into an empty state



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$$k_{B}T \ll E_{F}$$
 $I = \int_{E_{F}-eV}^{E_{F}} N_{L}(E)N_{R}(E+eV)T(E,V)[f(E)-f(E+eV)]dE$

2) $eV \ll \Phi$ $T(E,V) \approx T(E_F,0)$ Transmission factor independent on energy

3) $eV \ll E_F$ $N_R(E) \approx N_R(E_F)$

$$I = N_R(E_F)T(E_F, 0) \int_{E_F - eV}^{E_F} N_L(E)[f(E) - f(E + eV)]dE$$
 I is proportional to the integral of N_L in the interval E_F+eV

Measure I(V) to obtain N_L

$$\frac{dI}{dV} \propto \int_{E_F - eV}^{E_F} N_L(E) \left[-\frac{\partial f(E + eV)}{\partial (eV)} \right] dE$$





$$\frac{dI}{dV} \propto \int_{E_F - eV}^{E_F} N_L(E) \left[-\frac{\partial f(E + eV)}{\partial (eV)} \right] dE$$

Energy resolution strongly dependent on temperature

Typical Energy Resolution:

T=300 K $\Delta E = 0.1 eV$ 4.2 K $\Delta E \sim 1.5 meV$ 300 mK $\Delta E \sim 100 \mu eV$



$$\frac{dI}{dV} \propto N_L(E_F - eV) N_R(E_F)T(E_F, 0)$$

Differential conductance directly proportional to the density of states in the sample



T = 0 K

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Strong-coupling – details of electron-phonon coupling important

 Δ_k is complex and energy-dependent

 $\operatorname{Re}(\Delta_k) \Longrightarrow$ excitation energies

 $\operatorname{Im}(\Delta_k) \Rightarrow \operatorname{decay} \operatorname{of} \operatorname{qp} \operatorname{excitations}$ with the emission of phonons

Theory --- Eliashberg gap equation (1960) considered the retarded nature of electron-phonon coupling (not in BCS)

Results --- phonon modes $\Leftrightarrow N_S(E)$ variations

TWO
PARAMETERS $\left\{ \begin{array}{l} \mu^* \\ \alpha^2 F(\omega) \end{array} \right\}$ Coulomb pseudo-potential (repulsive interaction) $\alpha^2 F(\omega)$ electron-phonon (attractive interaction) $\alpha^2(\omega)$ electron-phonon coupling strength $F(\omega)$ phonon density of states



Bill McMillan

John Rowell

McMillan Conversion Procedure

$$\mu^*, \alpha^2 F \leftrightarrow N_S(E)$$
 iterative solution (vary $\mu^*, \alpha^2 F$)

$$T_c = \frac{\theta_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

where
$$\lambda = 2 \int_0^\infty d\omega \left(\frac{1}{\omega}\right) \alpha^2(\omega) F(\omega)$$

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Experiments (Rowell & McMillan) \rightarrow excellent agreement with known phonon data and fits to tunneling data





J. Scalapino, J. R. Schrieffer, and J. W. Wilkins, "Strong-coupling superconductivity. I," Physical Review, 148, 263 (1966).



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Strong-coupling – details of electron-phonon coupling important

Strong-coupling SC

Some superconductors

$$\frac{2\Delta(0)}{k_B T_c} > 3.53$$

Pb ~ 4.3, Nb ~ 4.8, Hg ~ 4.6, YBCO ~ 6

Structure in tunneling (for $eV \gg \Delta$)

For weak coupling $N(0)V \ll 1$, the details of the microscopic pairing wash out

For strong coupling $N(0)V \sim 1$, the details of the phonons responsible for the pairing are revealed



Structure near $k\theta_D$ (phonon frequencies)

Scanning Tunneling Microscope



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G. Binning & H. Rohrer (IBM, Zurich) Nobel Prize-1986

The Nobel Prize in Physics 1986 was divided, one half awarded to Ernst Ruska "for his fundamental work in electron optics, and for the design of the first electron microscope", the other half jointly to Gerd Binnig and Heinrich Rohrer "for their design of the scanning tunneling microscope."

Working Principle of the





Scanning Tunneling Microscope (STM) $I = N_R(E_F)T(E_F, 0) \int_{E_F-e_V}^{E_F} N_L(E)[f(E) - f(E + e_V)]dE$ WKB-approximation Barrier width $T(E_F, 0) \propto exp(-2\gamma)$ Barrier width $\gamma = \int_0^L \sqrt{\frac{2m\varphi}{\hbar^2}} dz = \frac{L}{\hbar} \sqrt{2m\varphi}$ Barrier height $\phi \approx \frac{\varphi_1 + \varphi_2}{2}$ Work functions $I \propto e^{-2kL} \int_{E_F}^{E_F} N_{sample}(E) [f(E) - f(E + eV)] dE$

> Main idea of the STM is to exploit the exponential decay of the tunneling current over the distance between tip and sample



Working Principle of the Scanning Tunneling Microscope (STM)

• Tunneling current

$$I \approx 18 \frac{V_s}{10000\Omega} \frac{k}{d} A_{eff} e^{-2kd} \qquad \qquad A_{eff} = \pi \times \left(\frac{1}{2} L_{eff}\right)^2 \\ L_{eff} \approx 2 \times \left[(R_t + d)/k \right]^{1/2}$$

2k [Å⁻¹]=1.025 $\Phi^{1/2}$ [eV]





What information can be accessed by STM/STS?



STM/STS

 $\frac{dI}{dV} \propto T(E_F) N_{Tip}(E_F) N_{sample}(E)$

NTUM



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300 mK STM Lab at Temple University



SOUNS A SUPERCONDUCTING QUANTUM

300 mK STM Lab at Temple University



STM Capabilities



Unisoku UHV-LT ³He Scanning Tunneling Microscope





Vortices in Superconductors



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Type I and Type II superconductors





Ginzburg-Landau Theory (1950)

order parameter
$$\psi(r) = \psi_0(r)e^{i\varphi(r)}$$

 $n_s = |\psi^*\psi| = \psi_0^2$



V. L. Ginzburg A. A. Abrikosov Nobel Prize in Physics 2003

Coherence length ξ is the length over which $\psi(r)$ changes appreciably



Ginzburg-Landau Theory (1950)

Free energy of the superconducting state:

$$g_{s}(T,H) = f_{n}(T,0) + \alpha |\psi|^{2} + \frac{\beta}{2} |\psi|^{4} + \frac{1}{2m^{*}} |(-i\hbar\nabla - e^{*}A)\psi|^{2} + \frac{1}{2\mu_{0}}B^{2} - B \bullet H$$

$$\begin{aligned} \alpha \psi + \beta \left|\psi\right|^2 \psi + \frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \vec{A}\right)^2 \psi &= 0\\ j_s &= \frac{e^* \hbar}{2m^* i} \left(\psi^* \nabla \psi - \psi \nabla \psi^*\right) - \frac{e^{*2}}{m^* c} \psi^* \psi \vec{A}\\ &= \frac{e^*}{m^*} \left|\psi\right|^2 \left(\hbar \nabla \phi - \frac{e^{*2}}{m^*} \vec{A}\right) = e^* \left|\psi\right|^2 \vec{v_s}\end{aligned}$$

$$\xi^2 = \frac{\hbar^2}{m^* |\alpha(T)|}$$
$$\lambda = \frac{m^*}{\mu_0 e^{*2} |\psi_0|^2}$$

L. P. Gor'kov, JETP 9, 1364(1959). A.A.Abrikosov, JETP 5, 1174(1957). ^{8/11/2023}

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Ginzburg-Landau theory (1950)

$$f_s = f_n + \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4$$

• For $\alpha < 0$, solve for minimum in $f_s - f_n \dots$

$$f_{s} - f_{n} = \alpha |\psi|^{2} + \frac{\beta}{2} |\psi|^{4}$$
$$\frac{d}{d|\psi|^{2}} (f_{s} - f_{n}) = \alpha + \beta |\psi|^{2} = 0$$
$$\implies |\psi_{\infty}|^{2} = \frac{-\alpha}{\beta}$$











elemental superconductors

	$\xi(nm)$	λ (nm)	T _c (K)	H _{e2} (1)
Al	1600	50	1.2	.01
Pb	83	39	7.2	.08
Sn	230	51	3.7	.03

predicted in 1950s by Abrikosov

	ξ (nm)	λ (nm)	$T_{c}(K)$	$H_{c2}(T)$
Nb ₃ Sn	11	200	18	25
YBCO	1.5	200	92	150
MgB_2	5	185	37	14



 $\mathcal{B}(\alpha),$

 $g_{\mu\nu}(t)$

Abrikosov Vortices in Superconductors

Type II superconducting sample in a magnetic field



What are vortices in superconductors?
Why are they important?
What can we learn from them?

How do we study and visualize them?



Single vortex

□ Has a core circled by supercurrents

Bogoliubov QPs are confined with the vortex core with size of ξ, leading to the vortex bound states.
 Outside the core there are superconducting electron pairs (Cooper pairs)





Phase Diagram of Type II Superconductors



 $H_{c1} \approx \frac{\Phi_0}{4\pi\lambda^2}$





Alex Abrikosov Nobel Prize in Physics 2003



Phase Diagram of High Tc Superconductors



In high Tc SC due to higher Tc, smaller x and high anisotropy thermal fluctuations are not negligible. Thermally induced vibrations of the flux lattice can melt it into a "vortex liquid".



How can we see vortices and what can we learn?





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Imaging of Vortices in Type II Superconductors

Magnetic Decoration



Order parameter and magnetic field profile of a single vortex



First image of Vortex lattice, 1967 Bitter Decoration Pb-4at%In rod, 1.1K, 195G U. Essmann and H. Trauble Physics Letters 24A, 526 (1967)



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How Vortices can be imaged by STM?

Tunneling conductance spectra in superconductor and normal metal

(b) σ_{N} 0 -3 З eV/∆



Conductance Maps at fixed energy



 $390 \text{ x} 390 \text{ nm}^2$

H=0.15 T T=1.5 K Nb Film Thickness=100 nm



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Determination of the coherence length



390 x 390 nm²



ξ = 15±1 nm

 $H_{c2} = 1.8 \text{ T}$



Different geometries and transitions of the Vortex LatticeNbSe2 $LuNi_2B_2C$



T= 4.2 K B=1.5 T

 $170 \text{ nm} \times 170 \text{ nm}$

The vortex lattice is oriented along the (110) direction of the crystal. Y. De Wilde, M. Iavarone, Phys. Rev. Lett. 78, 4273 (1997)

Shape of a single vortex: the case of $NbSe_2$



H. Hess *Phys. Rev. Lett.***62**, 214 (1989)

Gaps modulated in the ab-plane by the CDW I. Guillamon et al. PRB 77, 134505 (2008)



 $\Delta = \Delta_0 (1 + a \cos(6\varphi))$

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- Anisotropy of the superconducting gap
- Anisotropy of the Fermi surface
- Vortex lattice





 $v_F(\vec{k})$





Gap Anisotropy in borocarbides: YNi₂B₂C



 $\Delta(\mathbf{r})$ is fourfold-symmetric with the minima along the a-axis.

Nishimori et al., Journal of the Physical Society of Japan, 73 (12) 3247 (2004)



STM applied to Superconducting Qubits



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Nb Surface and Surface Treatments





Nb Thin Films- Local Gap Variation



Presence of Magnetic Moments



Time-reversal violated:

new states in the gap

 $JSN_0 \approx 1$

 $|JSN_0| \ll 1$

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Exchange interaction breaks pairs!

state in midgap

state near gap edge

 $E_0 \approx 0$

 $E_0 \approx \Delta_0$



Density of states

0.0

0.5

1.0

1.5

2.0

2.5

 $(JS\pi N_0/2)$

 $(JS\pi N_0)$

Kondo spin-flip tunneling



Shiba Bands



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ω/Δ Rusinov, A. I., 1968, Zh. Eksp. Teor. Fiz. Pis'ma Red. 9, 146 JETP Lett. 9,851969 Shiba, H₃₃1968, Prog. Theor. Phys. 40, 435. Yu, L., 1965, Acta Phys. Sin. 21, 75.

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 \mathcal{E}_0 =

A. V. Balatsky et al. , Rev. Modern Phys. 78, 373 (2006)

In-gap States





Conclusions

Measurements of the quasiparticle density of states spatially resolved (gap maps, localized and extended defects...)

- Usualization of vortices up to the upper critical field and allows to extract the superconducting coherence length ξ .
- Correlate superconducting parameters Δ , ξ with surface treatments and qubit measurements.





