PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Notes for Lecture 33

Continuation of introduction to the quantum theory of superconductivity

Bardeen, Cooper, Schrieffer, Phys. Rev. 108, 1175 (1957)

1. Summary of Fritz London's theory and of Cooper pair concept
2. Gap equation
3. Estimate of T_c
4. Comparison with London analysis

27	Fri: 04/08/2022		Multi electron atoms	[#21](#)	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	[#22](#)	04/18/2022
29	Wed: 04/13/2022		Multi electron atoms		
	Fri: 04/15/2022	*No class*	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons	[#23](#)	04/22/2022
31	Wed: 04/20/2022		Hubbard model with multiple electrons		
32	Fri: 04/22/2022		BCS model of superconductivity		
33	Mon: 04/25/2022		BCS model of superconductivity		
34	Wed: 04/27/2022		Review		
35	Fri: 04/29/2022		Review		

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

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Department of Physics, University of Illinois, Urbana, Illinois

(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°\text{K}$ to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

Some of you may wish to read the paper which is available from zsr.wfu.edu

https://doi.org/10.1103/PhysRev.108.1175

Overview of superconductivity --

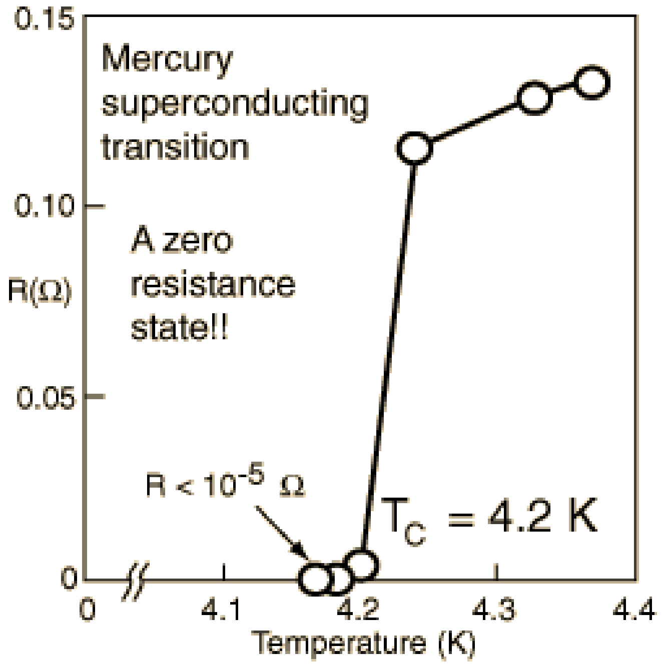
Ref:D. Teplitz, editor, Electromagnetism – paths to research, Plenum Press (1982); Chapter 1 written by Brian Schwartz and Sonia Frota-Pessoa

History:

1908 H. Kamerlingh Onnes successfully liquified He

1911 H. Kamerlingh Onnes discovered that Hg at 4.2 K has vanishing resistance

1957 Theory of superconductivity by Bardeen, Cooper, and Schrieffer



The surprising observation was that electrical resistivity abruptly dropped when the temperature of the material was lowered below a critical temperature T_c.

Some thoughts related to the statistical mechanics of Bose particles

For Bose particles, many particles can occupy the same state. This means that for non-interacting Bose particles, according to statistical mechanics, at very low temperature, it is possible for a macroscopic number of particles to occupy the lowest single particle state and produce a "Bose condensate". ^{4}He is not a good example of this, since the particles have significant interactions, but the superfluid behavior is logically related. A better example was demonstrated in 1995 with 2.5 x 10^{12} ^{87}Rb atoms cooled to 1.7 x 10^{-7}K.

For superconductivity, electrons are the particles. How is possible for Fermi particles to behave with Bose-like statistics?

Introduced the notion of a Cooper pair of electrons that behave somewhat like electrons and that are stabilized by an attractive interaction.

Some phenomenological theories < 1957 thanks to F. London

Drude model of conductivity in "normal" materials

$$m\frac{d\mathbf{v}}{dt} = -e\mathbf{E} - m\frac{\mathbf{v}}{\tau}$$

$$\mathbf{v}(t) = \mathbf{v}_0 e^{-t/\tau} - \frac{e\mathbf{E}\tau}{m}$$

$$\mathbf{J} = -ne\mathbf{v}; \qquad \text{for } t >> \tau \qquad \Rightarrow \qquad \mathbf{J} = \frac{ne^2\tau}{m}\mathbf{E} \equiv \sigma\mathbf{E}$$

Note: Equations are in cgs Gaussian units.

London model of conductivity in superconducting materials; $\tau \rightarrow \infty$

$$m\frac{d\mathbf{v}}{dt} = -e\mathbf{E}$$

$$\frac{d\mathbf{v}}{dt} = -\frac{e\mathbf{E}}{m} \qquad\qquad \frac{d\mathbf{J}}{dt} = -ne\frac{d\mathbf{v}}{dt} = \frac{ne^2\mathbf{E}}{m}$$

From Maxwell's equations:

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$$

London model of conductivity in superconducting materials; $\tau \rightarrow \infty$

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Some phenomenological theories < 1957

London model of conductivity in superconducting materials

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From Maxwell's equations:

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} \qquad \nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \left(\nabla \times \mathbf{B}\right) = -\nabla^2\mathbf{B} = \frac{4\pi}{c}\nabla \times \mathbf{J} - \frac{1}{c^2}\frac{\partial^2 \mathbf{B}}{\partial t^2}$$

$$-\nabla^2\frac{\partial \mathbf{B}}{\partial t} = \frac{4\pi}{c}\nabla \times \frac{\partial \mathbf{J}}{\partial t} - \frac{1}{c^2}\frac{\partial^3 \mathbf{B}}{\partial t^3}$$

$$-\nabla^2\frac{\partial \mathbf{B}}{\partial t} = \frac{4\pi ne^2}{mc}\nabla \times \mathbf{E} - \frac{1}{c^2}\frac{\partial^3 \mathbf{B}}{\partial t^3}$$

$$-\nabla^2\frac{\partial \mathbf{B}}{\partial t} = -\frac{4\pi ne^2}{mc^2}\frac{\partial \mathbf{B}}{\partial t} - \frac{1}{c^2}\frac{\partial^3 \mathbf{B}}{\partial t^3}$$

$$\frac{\partial}{\partial t}\left(\nabla^2 - \frac{1}{\lambda_L^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{B} = 0 \qquad \text{with } \lambda_L^2 \equiv \frac{mc^2}{4\pi ne^2}$$

London model – continued

London model of conductivity in superconducting materials

$$\frac{d\mathbf{J}}{dt} = -ne\frac{d\mathbf{v}}{dt} = \frac{ne^2\mathbf{E}}{m}$$

$$\frac{\partial}{\partial t}\left(\nabla^2 - \frac{1}{\lambda_L^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{B} = 0 \qquad \text{with } \lambda_L^2 \equiv \frac{mc^2}{4\pi ne^2}$$

For slowly varying solution:

$$\frac{\partial}{\partial t}\left(\nabla^2 - \frac{1}{\lambda_L^2}\right)\mathbf{B} = 0 \qquad \text{for } \frac{\partial \mathbf{B}}{\partial t} = \hat{\mathbf{z}}\frac{\partial B_z(x,t)}{\partial t}:$$

$$\Rightarrow \frac{\partial B_z(x,t)}{\partial t} = \frac{\partial B_z(0,t)}{\partial t}e^{-x/\lambda_L}$$

Here we assume we know the boundary value at *x=0*.

London's leap: $B_z(x,t) = B_z(0,t)e^{-x/\lambda_L}$

Consistent results for current density:

$$\frac{4\pi}{c}\nabla\times\mathbf{J} = -\nabla^2\mathbf{B} = -\frac{1}{\lambda_L^2}\mathbf{B} \qquad \mathbf{J} = \hat{\mathbf{y}}J_y(x) \qquad \Rightarrow \quad J_y(x) = \lambda_L\frac{ne^2}{mc}\mathrm{B}_z(0)\,\mathrm{e}^{-\mathrm{x}/\lambda_L}$$

London model – continued

Penetration length for superconductor: $\lambda_L^2 \equiv \frac{mc^2}{4\pi ne^2}$ Typically, $\lambda_L \approx 10^{-7}\, m$

$B_z(x,t) = B_z(0,t)e^{-x/\lambda_L}$

Vector potential for $\mathbf{B} = \nabla \times \mathbf{A}$ and $\nabla \cdot \mathbf{A} = 0$:

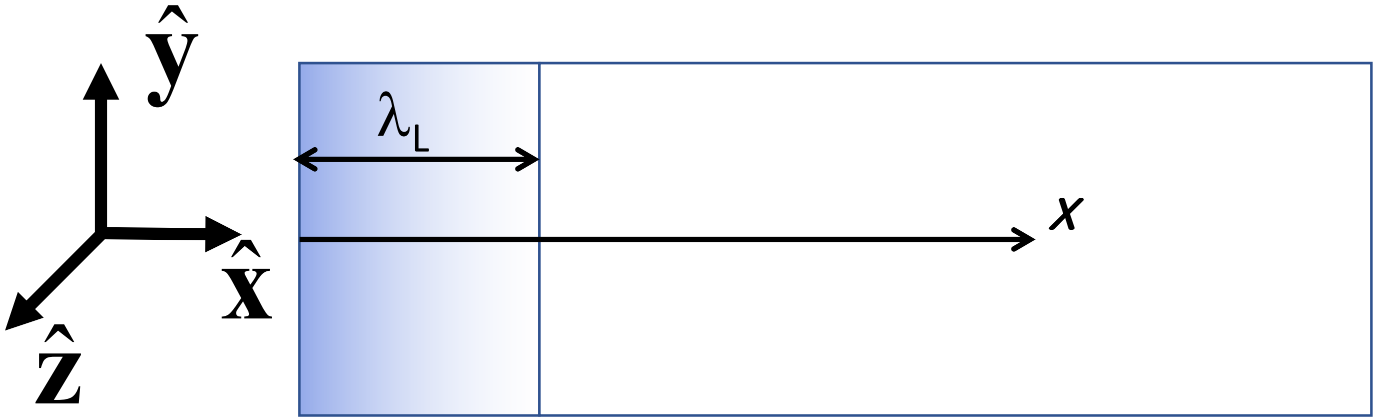
$\mathbf{A} = \hat{\mathbf{y}} A_y(x)$ $\qquad A_y(x) = -\lambda_L B_z(0) e^{-x/\lambda_L}$

Note that: $\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J}$

$-\nabla^2 \mathbf{A} = \frac{4\pi}{c}\mathbf{J} \;\Rightarrow \nabla^2 \mathbf{A} + \frac{4\pi}{c}\mathbf{J} = 0$

Recall form for current density: $J_y(x) = \lambda_L \frac{ne^2}{mc} \mathrm{B}_z(0)\, \mathrm{e}^{-x/\lambda_L}$

$\Rightarrow \mathbf{J} + \frac{ne^2}{mc}\mathbf{A} = 0$ or $\frac{ne}{m}\left(m\mathbf{v} + \frac{e}{c}\mathbf{A}\right) = 0$



Challenge for BSC –

What is the microscopic origin of this two-electron current and why is it stable at low temperature?

Using creation/annihilation operators for Bloch eigenstates:

Bloch states specified by wave vector **k** and spin σ, which satisfy the usual Fermi commutation relations:

$$[c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}{}^*]_+ = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}, \qquad (2.1)$$

$$[c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}]_+ = 0. \qquad (2.2)$$

The single-particle number operator $n_{\mathbf{k}\sigma}$ is defined as

$$n_{\mathbf{k}\sigma} = c_{\mathbf{k}\sigma}{}^* c_{\mathbf{k}\sigma}. \qquad (2.3)$$

From these single particle states, form Cooper pair states

We start then by considering a reduced problem in which we include only configurations in which the states are occupied in pairs such that if **k**↑ is occupied so is −**k**↓. A pair is designated by the wave vector **k**, independent of spin. Creation and annihilation operators for pairs may be defined in terms of the single-particle operators as follows:

$$b_{\mathbf{k}}=c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}, \qquad (2.9)$$

$$b_{\mathbf{k}}^*=c_{\mathbf{k}\uparrow}^*c_{-\mathbf{k}\downarrow}^*. \qquad (2.10)$$

These operators satisfy the commutation relations

$$[b_{\mathbf{k}},b_{\mathbf{k}'}^*]_-=(1-n_{\mathbf{k}\uparrow}-n_{-\mathbf{k}\downarrow})\delta_{\mathbf{k}\mathbf{k}'}, \qquad (2.11)$$

$$[b_{\mathbf{k}},b_{\mathbf{k}'}]_-=0, \qquad (2.12)$$

$$[b_{\mathbf{k}},b_{\mathbf{k}'}]_+=2b_{\mathbf{k}}b_{\mathbf{k}'}(1-\delta_{\mathbf{k}\mathbf{k}'}), \qquad (2.13)$$

where $n_{\mathbf{k}\sigma}$ is given by (2.3). While the commutation relation (2.12) is the same as for bosons, the commutators (2.11) and (2.13) are distinctly different from those for Bose particles. The factors $(1-n_{\mathbf{k}\uparrow}-n_{-\mathbf{k}\downarrow})$ and $(1-\delta_{\mathbf{k}\mathbf{k}'})$ arise from the effect of the exclusion principle on the single particles.

The BCS Hamiltonian takes the form:

$$H_{\mathrm{red}}=2\sum_{k>k_F}\epsilon_{\mathbf{k}}b_{\mathbf{k}}^*b_{\mathbf{k}}+2\sum_{k<k_F}|\epsilon_{\mathbf{k}}|b_{\mathbf{k}}b_{\mathbf{k}}^*-\sum_{\mathbf{k}\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}b_{\mathbf{k}'}^*b_{\mathbf{k}}. \qquad (2.14)$$

The BCS Hamiltonian takes the form:

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Single particle energy Relative to ε_F

Attractive interaction potential due to electron-phonon interaction

Form of variational wavefunction:

$$\Psi=\prod_{\mathbf{k}}[(1-h_{\mathbf{k}})^{\frac{1}{2}}+h_{\mathbf{k}}^{\frac{1}{2}}b_{\mathbf{k}}^*]\Phi_0, \qquad (2.16)$$

Here the variational parameters h_k represent the probability that pair state k is occupied.

Evaluating the matrix elements --

$$\langle \Psi | H | \Psi \rangle =$$

$$W_0 = W_{KE} + W_I = 2 \sum_{k>k_F} \epsilon_{\mathbf{k}} h_{\mathbf{k}} + 2 \sum_{k<k_F} |\epsilon_{\mathbf{k}}| (1 - h_{\mathbf{k}}) - \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} [h_{\mathbf{k}}(1-h_{\mathbf{k}}) h_{\mathbf{k}'}(1-h_{\mathbf{k}'})]^{\frac{1}{2}}. \quad (2.32)$$

Optimizing the energy with respect to the variational parameters:

$$\frac{[h_{\mathbf{k}}(1-h_{\mathbf{k}})]^{\frac{1}{2}}}{1-2h_{\mathbf{k}}} = \frac{\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} [h_{\mathbf{k}'}(1-h_{\mathbf{k}'})]^{\frac{1}{2}}}{2\epsilon_{\mathbf{k}}}. \quad (2.33)$$

Simplification for $V_{kk'}$:

$$V_{kk'} = \begin{cases} V & \text{for } -\hbar\omega \le \varepsilon_k \le \hbar\omega \\ 0 & \text{otherwise} \end{cases}$$

Introduction of the average matrix element into (2.33) leads to

$$h_{\mathbf{k}}=\frac{1}{2}\left[1-\frac{\epsilon_{\mathbf{k}}}{(\epsilon_{\mathbf{k}}^2+\epsilon_0^2)^{\frac{1}{2}}}\right], \tag{2.35}$$

and

$$[h_{\mathbf{k}}(1-h_{\mathbf{k}})]^{\frac{1}{2}}=\frac{\epsilon_0}{2(\epsilon_{\mathbf{k}}^2+\epsilon_0^2)^{\frac{1}{2}}}, \tag{2.36}$$

where

$$\epsilon_0=V\sum_{\mathbf{k}'}[h_{\mathbf{k}'}(1-h_{\mathbf{k}'})]^{\frac{1}{2}}, \tag{2.37}$$

the sum extending over states within the range $|\epsilon_{\mathbf{k}}| < \hbar\omega$. If (2.36) and (2.37) are combined, one obtains a condition on ϵ_0:

$$\frac{1}{V}=\sum_{\mathbf{k}}\frac{1}{2(\epsilon_{\mathbf{k}}^2+\epsilon_0^2)^{\frac{1}{2}}}. \tag{2.38}$$

Replacing the sum by an integral and recalling that $V=0$ for $|\epsilon_{\mathbf{k}}|>\hbar\omega$, we may replace this condition by

$$\frac{1}{N(0)V}=\int_0^{\hbar\omega}\frac{d\epsilon}{(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}}. \tag{2.39}$$

Solving for ϵ_0, we obtain

$$\epsilon_0=\hbar\omega\Big/\sinh\left[\frac{1}{N(0)V}\right]. \tag{2.40}$$

where $N(0)$ is the density of Bloch states of one spin per unit energy at the Fermi surface.

The ground state energy is obtained by combining the expressions for $h_{\mathbf{k}}$ and ϵ_0, (2.35), (2.36), and (2.37), with (2.32). We find

$$W_0 = 4N(0)\int_0^{\hbar\omega} \epsilon h(\epsilon)d\epsilon - \frac{{\epsilon_0}^2}{V}$$

$$= 2N(0)\int_0^{\hbar\omega}\left[\epsilon - \frac{\epsilon^2}{(\epsilon^2+{\epsilon_0}^2)^{\frac{1}{2}}}\right]d\epsilon - \frac{{\epsilon_0}^2}{V}, \quad (2.41)$$

where we have used the fact that $[1-h(-\epsilon)]=h(\epsilon)$, that is, the distribution function is symmetric in electrons and holes with respect to the Fermi surface.

At 0K, the energy difference of the superconducting state relative to the "normal" state is:

$$W_0 = N(0)(\hbar\omega)^2\left\{1-\left[1+\left(\frac{\epsilon_0}{\hbar\omega}\right)^2\right]^{\frac{1}{2}}\right\} = \frac{-2N(0)(\hbar\omega)^2}{e^{[2/N(0)V]}-1}.$$

(2.42)

Ground state of BCS Hamiltonian at 0 K --

$$W_0 = N(0)(\hbar\omega)^2\left\{1-\left[1+\left(\frac{\epsilon_0}{\hbar\omega}\right)^2\right]^{\frac{1}{2}}\right\} = \frac{-2N(0)(\hbar\omega)^2}{e^{[2/N(0)V]}-1}. \quad (2.42)$$

Considering excitations to this ground state – BCS Hamiltonian has a energy gap of $2\varepsilon_0$

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega} \frac{d\epsilon}{(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}} \tanh\left[\tfrac{1}{2}\beta(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}\right], \quad (3.27) \qquad \text{where} \quad \beta = \frac{1}{k_B T}$$

The transition temperature T_c can be estimated as the solution when $\varepsilon_0 = 0$.

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega} \frac{d\epsilon}{\epsilon} \tanh\left(\tfrac{1}{2}\beta_c\epsilon\right) \Rightarrow kT_c = 1.14\hbar\omega \exp\left[-\frac{1}{N(0)V}\right]$$

For $k_B T_c \ll \hbar\omega$

Plot of gap parameter as a function of temperature --

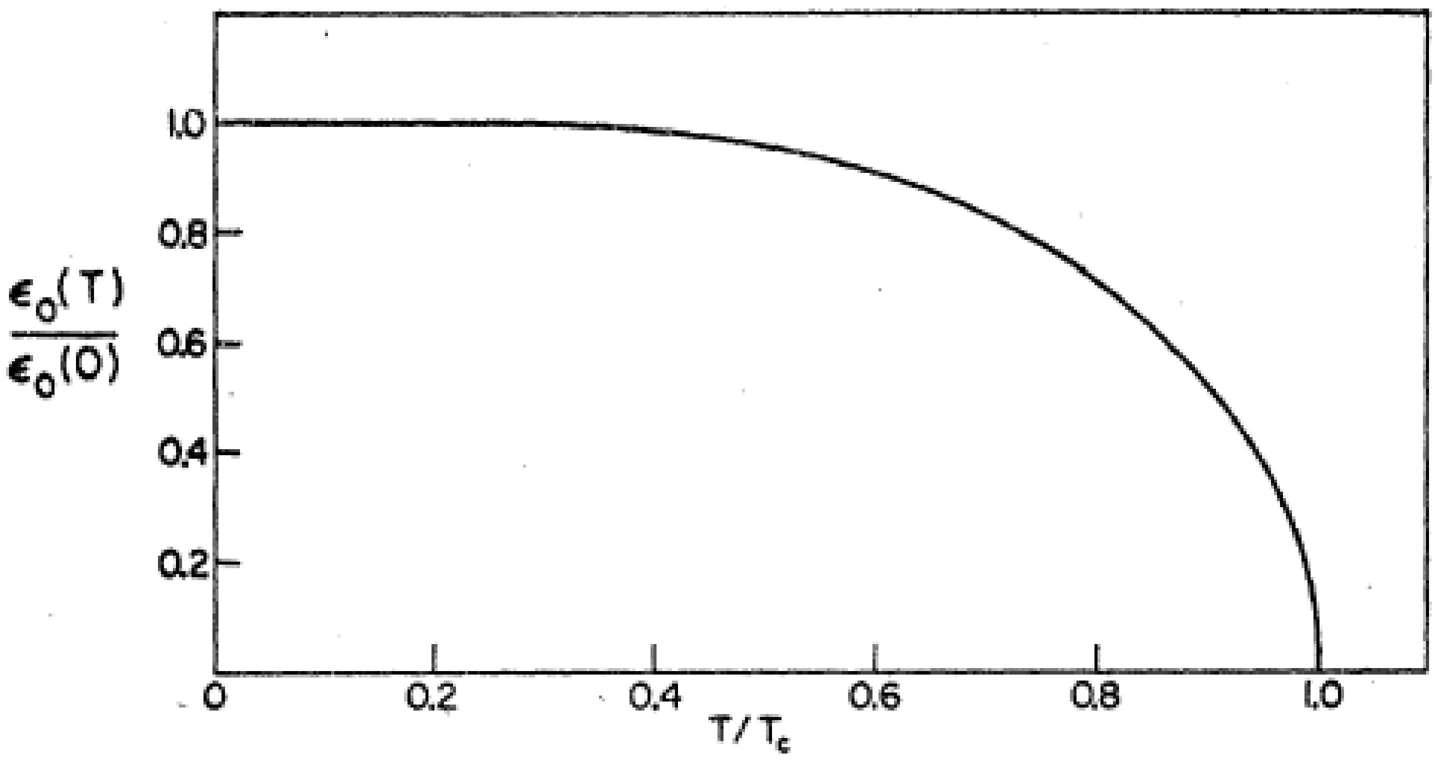

FIG. 1. Ratio of the energy gap for single-particle-like excitations to the gap at $T = 0°K$ *vs* temperature.

This treatment has assumed that there are no magnetic fields present in the system. An applied magnetic field can also affect superconductivity.

The critical field for a bulk specimen of unit volume is given by

$$H_c^2/8\pi = F_n - F_s, \tag{3.32}$$

where F_n is the free energy of the normal state:

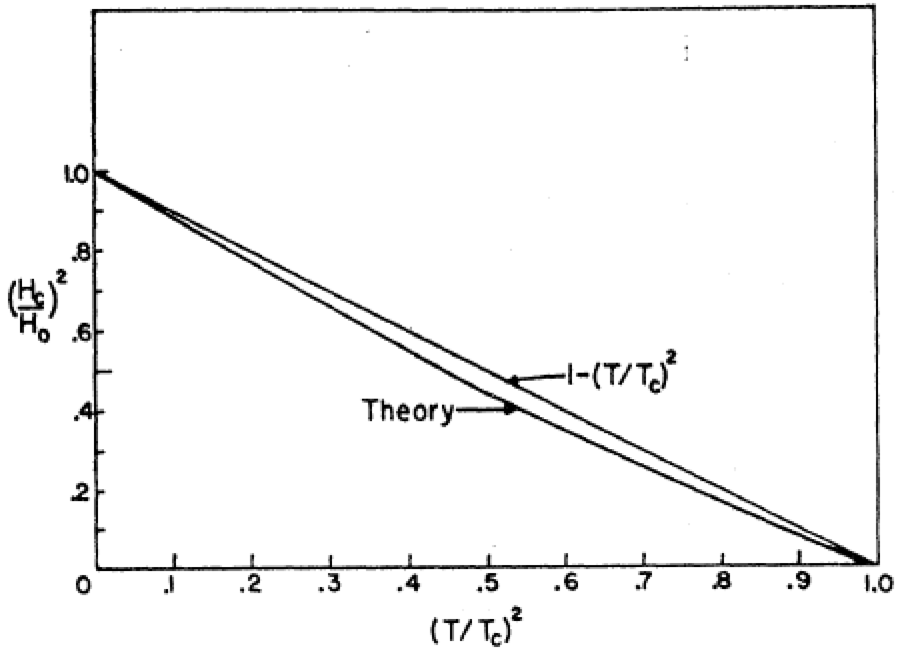

FIG. 2. Ratio of the critical field to its value at $T=0°K$ *vs* $(T/T_c)^2$. The upper curve is the $1-(T/T_c)^2$ law of the Gorter-Casimir theory and the lower curve is the law predicted by the theory in the weak-coupling limit. Experimental values generally lie between the two curves.

Superconducting current –

Single particle Bloch wavefunctions --

We expand ψ and ψ^* in creation and annihilation operators[36]:

$$\psi(\mathbf{r}) = \frac{1}{\Omega^{\frac{1}{2}}} \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} u_\sigma e^{i\mathbf{k}\cdot\mathbf{r}},$$
$$\psi^*(\mathbf{r}) = \frac{1}{\Omega^{\frac{1}{2}}} \sum_{\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma'}^* u_{\sigma'}^* e^{-i\mathbf{k}'\cdot\mathbf{r}}, \tag{5.6}$$

where the c's satisfy the usual fermion anticommutation relations, (2.1) and (2.2), u_σ is a two-component spinor, and Ω is the volume of the container. The interaction

$$\mathfrak{J}(\mathbf{r}) = \frac{ie\hbar}{2m}(\psi^*\nabla\psi - \text{Herm. conj.}) - \frac{e^2}{mc}\psi^*\mathbf{A}\psi$$
$$= \mathfrak{J}_P(\mathbf{r}) + \mathfrak{J}_D(\mathbf{r})$$

The paramagnetic contribution is complicated, but is generally small at low temperature.

However, the diamagnetic term: $$\mathbf{j}_D(\mathbf{r}) = -(ne^2/mc)\mathbf{A}(\mathbf{r}), \tag{5.14}$$

is significant and is consistent with the London expression.

BCS estimate of penetration depth --

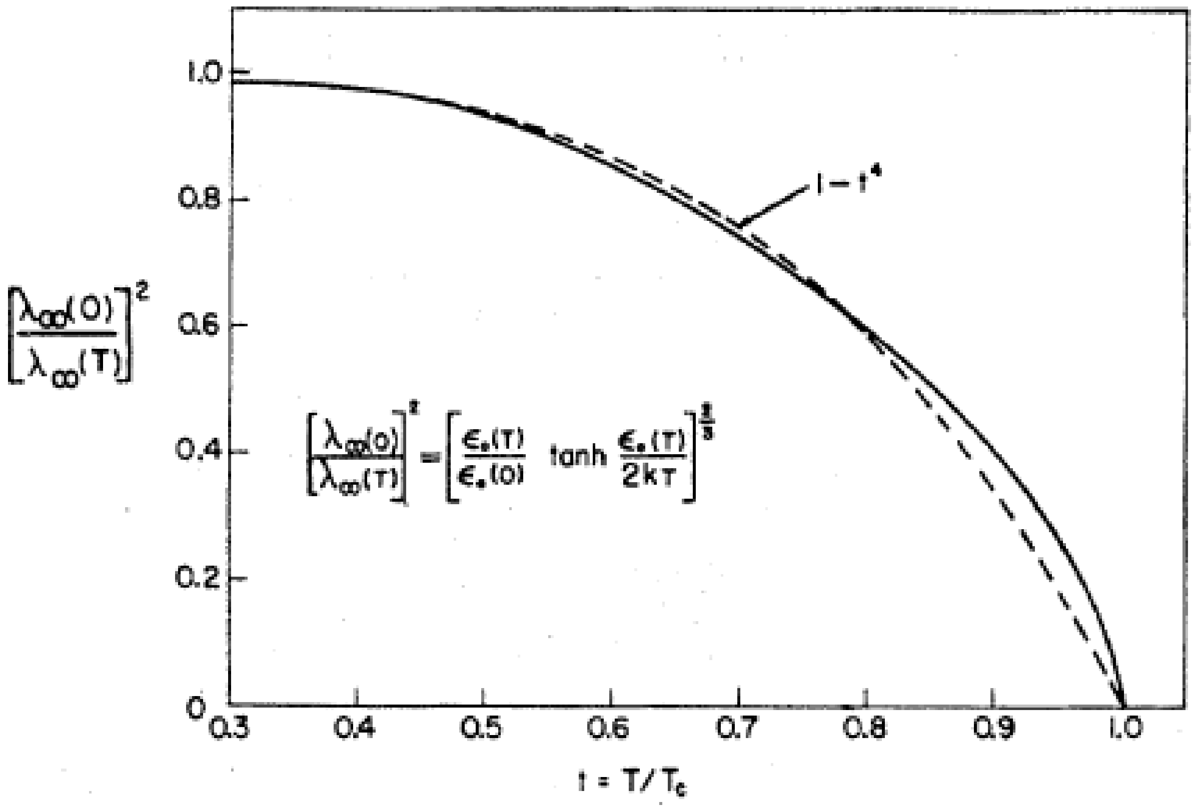

FIG. 6. The temperature variation of the penetration depth, λ_∞, in the infinite coherence distance limit, $(\xi_0/\lambda)\rightarrow\infty$, compared with the empirical law, $[\lambda(0)/\lambda(T)]^2 = 1-t^4$.