

CHAPTER V

THERMAL CONDUCTIVITY

V.1 Mechanisms of Thermal Conductivity

The heat flux in a metal is composed of two components; the electronic thermal conductivity and the thermal conductivity of the lattice. As the temperature is reduced below T_c the electronic conductivity becomes smaller than in the normal state, while the lattice component rises steadily and becomes the dominant component at temperatures well below T_c . The physical reasons for these features have been first recognized and understood by Mendelssohn and Renton⁽²²⁾ with the supposition that the superconductive electrons carry no entropy (which is derived from the fact that a superconductor has no Thomson heat), and therefore give no contribution to the transport of heat. Thus the electronic conductivity of the metal will progressively decrease towards lower temperatures. Since at low enough temperatures the concentration of normal electrons will be negligibly small, the heat conduction of the metal in this region may be entirely due to the lattice waves. From the experimental evidence available these authors also concluded that as superconductivity is established, interaction between electrons and lattice vibrations disappears. It might therefore be expected that in a superconductor, corresponding to the decrease of the electronic conduction, an increase in the lattice conductivity will take place owing to the increased

phonon mean free path. Near absolute zero the heat conductivity of a superconductor should therefore depart completely from ordinary metallic behavior and present the same aspect as that of a dielectric. Base on BCS theory Bardeen, Rickayzen, and Tewordt⁽²³⁾ worked out the magnitude and temperature dependence of the lattice and electronic conductivity in the superconducting state.

V.2 Kubo's formulas for the Transport Coefficients

The transport coefficient can be defined as:⁽²⁴⁾

$$j = -\frac{\mu}{\ell} L_0 \left(\frac{1}{\mu} \nabla \mu - \frac{1}{T} \nabla T \right) - L_1 \frac{1}{T} \nabla T, \quad (5.1)$$

$$u = -\frac{\mu}{\ell} L_1 \left(\frac{1}{\mu} \nabla \mu - \frac{1}{T} \nabla T \right) - L_2 \frac{1}{T} \nabla T, \quad (5.2)$$

where j is the electrical current density and u is the energy flux. T is the temperature and μ the chemical potential. Then the transport coefficients, L_i , are given by the Kubo formulas:⁽¹¹⁾

$$L_0 = \frac{1}{3\Omega} \int_0^\infty dt \int_0^\beta d\lambda \text{Tr} [\rho_0 J(0) \cdot J(t+i\lambda)], \quad (5.3)$$

$$L_1 = \frac{1}{3\Omega} \int_0^\infty dt \int_0^\beta d\lambda \text{Tr} [\rho_0 U(0) \cdot J(t+i\lambda)] \\ = \frac{1}{3\Omega} \int_0^\infty dt \int_0^\beta d\lambda \text{Tr} [\rho_0 J(0) \cdot U(t+i\lambda)], \quad (5.4)$$

$$L_2 = \frac{1}{3\Omega} \int_0^\infty dt \int_0^\beta d\lambda \text{Tr} [\rho_0 U(0) \cdot U(t+i\lambda)]. \quad (5.5)$$

Here, J and U are the Heisenberg operators for the total electrical and energy currents, respectively. ρ_0 is the equilibrium density matrix:

$$\rho_0 = \frac{1}{Z} \exp[-\beta(H - \mu N)] ,$$

$$Z = \text{Tr} \exp[-\beta(H - \mu N)] ,$$

where H is the Hamiltonian for the system and N is the number operator. $\beta = 1/k_B T$, and Ω is the volume of the system.

If there is no temperature gradient, $\nabla \mu = -eE$, where E is the external electric field, then we may identify the dc conductivity σ with L_0 :

$$L_0 = \sigma . \quad (5.7)$$

The heat flux q is given by

$$q = u - \frac{\mu}{e} j . \quad (5.8)$$

From the definition of the thermal conductivity, K ,

$$q = -K \nabla T , \quad j = 0 \quad (5.9)$$

then the thermal conductivity can be defined as

$$K = \frac{1}{T} (L_2 - \frac{L_1^2}{L_0}) , \quad (5.10)$$

In evaluating the right-hand side of Eq.(5.10), the major difficulty is that we are required to compute the L 's to order T^2 in order to obtain a non-vanishing result.

V.3 Calculation of the Thermal Conductivity

Our starting point will be the Kubo formula for thermal conductivity as derived by Luttinger⁽²⁵⁾ in a homogeneous system.

In order to obtain a rigorous derivation, he does not introduce the usual Hamiltonian describing the variation of temperature, but computes the linear response to a gravitational field which in principle produces energy flow and temperature fluctuations. But we are interested in the flow of energy with no flow of matter. To avoid infinity when the system becomes superconducting, he discusses some new equations and derives directly the thermal conductivity in terms of the correlation function of current density in the unperturbed system.

For the thermal conductivity we are interested in the flow of energy with no flow of matter. We shall neglect terms of order $(k_B T / \mu)$, and we can verify that to this order the matter current accompanying an energy current is reduced to zero by measuring energies with respect to the chemical potential. The Kubo formula for the thermal conductivity K may be written as follows (we use units in which $\hbar = 1$):

$$K = \frac{2}{3VT} \int_{-\infty}^{\infty} t_2 dt_2 \int d^3x_1 d^3x_2 \langle u(x_1, 0) \cdot u(x_2, t_2) \rangle. \quad (5.11)$$

Above V is the volume of the system, T is the temperature, and u is the heat-current density operator at the space-time point (x_1, t_1) . The brackets denote an average in the grand canonical ensemble. If we write the Hamiltonian for the system in terms of the annihilation and creation operators $\psi_{\delta}^{\dagger}(x)$ and $\psi_{\delta}(x)$, the heat current density operator has the form

$$u(x) = -\frac{i}{2m} \sum_{\delta} \left(\dot{\psi}_{\delta}^{\dagger}(x) \cdot \nabla \psi_{\delta}(x) + \nabla \psi_{\delta}^{\dagger}(x) \cdot \dot{\psi}_{\delta}(x) \right), \quad (5.12)$$

obeys the heat equation

$$\dot{h}(x) + \nabla \cdot u(x) = 0, \quad (5.13)$$

where $h(x)$ is the Hamiltonian density of the system.

It is convenient to introduce the correlation function

$$P(1,2) = \langle T [u(1) \cdot u(2)] \rangle, \quad (5.14)$$

where 1,2 denote space-time points, and T is Wick's time ordering operator. In the standard way we make Fourier transformations in the spatial and imaginary time difference coordinates, so that

$$P(1,2) = i k_B T \sum_{\nu_m} \int \frac{d^3 q}{(2\pi)^3} P(\vec{q}, \nu_m) \exp\{i q \cdot (x_1 - x_2) - i \nu_m (t_1 - t_2)\}. \quad (5.15)$$

Here $\nu_m = 2\pi m i / \beta$ and $\beta = (k_B T)^{-1}$; m running over all integers. In terms of $P(\vec{q}, \nu_m)$ Eq.(5.14) becomes

$$K = \frac{1}{6T} \lim_{\omega \rightarrow 0} \frac{P(\vec{q}=0, \nu_m = \omega + i0^+) - P(\vec{q}=0, \nu_m = \omega - i0^+)}{\omega}. \quad (5.16)$$

It is convenient to use Nambu's two component field operators⁽²⁶⁾ defined by

$$\Psi_{(1)} = \begin{pmatrix} \Psi_{\uparrow}^{(1)} \\ \Psi_{\downarrow}^{(1)} \end{pmatrix}, \quad \Psi_{(1)}^+ = (\Psi_{\uparrow}^{+(1)} \quad \Psi_{\downarrow}^{+(1)}).$$

In terms of these and the Pauli spin matrices \mathcal{J}_i the correlation function may be written as follows

$$P(1,2) = \frac{1}{4m^2} \left(\frac{\partial}{\partial t_1} \nabla_1 + \frac{\partial}{\partial t_1} \nabla_1 \right) \left(\frac{\partial}{\partial t_2} \nabla_2 + \frac{\partial}{\partial t_2} \nabla_2 \right) (\mathcal{J}_3)^{ij} (\mathcal{J}_3)^{kl} \\ \times \langle T [\Psi_i^{(1)} \Psi_k^{(2)} \Psi_{\ell}^{+(2')} \Psi_j^{+(1')}] \rangle \Big|_{\substack{i'=1 \\ j'=2}} \quad (5.17)$$

Where in writing the correlation function in the above form, we have neglected the discontinuity terms that arise from the derivatives acting on the time ordering operator. These terms do not contribute to the thermal conductivity.

By using the Hartree-Fock approximation, the T product of four operators is

$$\langle T[\Psi_i(1)\Psi_k(2)\Psi_l^+(2')\Psi_j^+(1')] \rangle \rightarrow G_{il}(1,2')G_{kj}(2,1'), \quad (5.18)$$

where $G_{il}(1,2)$ is Nambu's matrix Green's function:

$$G_{il}(1,2) = -i \langle T[\Psi_i(1)\Psi_l^+(2)] \rangle. \quad (5.19)$$

Then we obtain from Eqs. (5.17), (5.18), and (5.15)

$$\begin{aligned} P(\vec{q}, \nu_m) &= \frac{i}{\beta} \sum_{\mathcal{J}_l} \int \frac{d^3p}{(2\pi)^3} e^{\mathcal{J}_l 0^+} \left[\mathcal{J}_l(\vec{p} + \vec{q}) + (\mathcal{J}_l + \nu_m)\vec{p} \right]^2 \\ &\times \frac{1}{4m^2} \text{Tr} \left[\mathcal{J}_3 G(\vec{p} + \vec{q}; \mathcal{J}_l + \nu_m) \mathcal{J}_3 G(\vec{p}; \mathcal{J}_l) \right], \end{aligned} \quad (5.20)$$

where $\mathcal{J}_l = (2l+1)\pi i/\beta$ and l takes on integral values.

We now insert the spectral representation for $G(\vec{p}, \mathcal{J}_l)$,

$$G(\vec{p}, \mathcal{J}_l) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{a(\vec{p}, \omega)}{\mathcal{J}_l - \omega}, \quad (5.21)$$

where the spectral function $a(\vec{p}, \omega)$ is obtained from

$$\begin{aligned} a(\vec{p}, \omega) &= 2 \text{Im} G(\vec{p}, \omega - i0^+) \\ &= \frac{1}{i} [G(\vec{p}, \omega - i0^+) - G(\vec{p}, \omega + i0^+)]. \end{aligned} \quad (5.22)$$

Substituting Eq.(5.21) into(5.20) and do the $\sum_{\mathbf{q}}$ sum, then the thermal conductivity is

$$K = \frac{1}{24m^2k_B T^2} \int \frac{d^3p d\omega}{(2\pi)^4} p^2 \omega^2 \operatorname{sech}^2\left(\frac{1}{2}\beta\omega\right) \left[\operatorname{Tr} \left\{ \mathcal{T}_3^{\dagger} a(\mathbf{p}, \omega) \mathcal{T}_3 a(\mathbf{p}, \omega) \right\} \right]. \quad (5.23)$$

We still must decide which Green's function, the s-electron Green's function or the d-electron Green's function, should be used in formula(5.23). If we use the d-electron Green's function, then the carrier of the heat current would be the d-electrons. However if the s-electrons are to be the carrier of the heat current, then the s-electron wave functions should be used in(5.23). For transition metals in the normal state, the choice is obvious since the s-electrons are the carriers. To decide which electrons are the carriers of the heat current when the transition metal is in the superconducting state, we must remember that only normal electrons can contribute to the heat current since the superconducting electrons do not carry any entropy. Since the normal d-electrons are not the carriers of the heat current in the first place, their transformation into super d-electrons should not cause the observed decrease in the thermal current. The decrease in the heat current can only be accounted for by a change in the number of normal s-electrons (these being the carriers of the heat current). For this reason we believe that the s-electron Green's functions must be used in the thermal conductivity formula(5.23).

V.4 Analytical Treatment

The integral over momenta in Eq(5.23) can be converted into one over ϵ . Now let's consider the spectral function $a(\vec{p}, \omega)$. We have the Green's function for s-electrons as in Eq.(4.26) of chapter IV, i.e.,

$$G(\epsilon, \omega) = \frac{1}{\text{Det } G^{-1}} \begin{pmatrix} \omega + \epsilon - \frac{V^2}{2\pi} M_{22} & \frac{V^2}{2\pi} M_{12} \\ \frac{V^2}{2\pi} M_{21} & \omega - \epsilon - \frac{V^2}{2\pi} M_{11} \end{pmatrix},$$

where

$$\text{Det } G^{-1} = \left(\omega - \epsilon - \frac{V^2}{2\pi} M_{11} \right) \left(\omega + \epsilon - \frac{V^2}{2\pi} M_{22} \right) - \frac{V^4}{4\pi^2} M_{12} M_{21}.$$

Here we use the notation $\sum_j |V_{kj}|^2 = V^2$

We consider first the numerator of $G(\epsilon, \omega)$, the numerator of $\text{Tr} \{ \mathcal{I}_3 G(\epsilon, \omega) \mathcal{I}_3 G(\epsilon, \omega) \}$ is then

$$\left(\omega + \epsilon - \frac{V^2}{2\pi} M_{22} \right)^2 + \left(\omega - \epsilon - \frac{V^2}{2\pi} M_{11} \right)^2 - \frac{2V^4}{4\pi^2} M_{12} M_{21}.$$

Let

$$Q = \frac{V^2}{2\pi} M_{11},$$

$$R = \frac{V^2}{2\pi} M_{22},$$

$$\Delta' = \frac{V^4}{4\pi^2} M_{12} M_{21},$$

$$\text{then } Q - R = -\frac{NV^2}{\pi} \frac{B}{(\Delta_g^2 + B^2 - \omega^2)}, \quad (5.24)$$

$$Q + R = -\frac{NV^2}{\pi} \frac{\omega}{(\Delta_g^2 + B^2 - \omega^2)}, \quad (5.25)$$

$$QR = -\frac{N^2 V^4}{4\pi^2} \frac{\omega^2 + B^2}{(\Delta_g^2 + B^2 - \omega^2)}. \quad (5.26)$$

And the numerator of $\text{Tr} \{ \mathcal{J}_3 G(\epsilon, \omega) \mathcal{J}_3 G(\epsilon, \omega) \}$ becomes

$$\begin{aligned} & (\omega - \epsilon - Q)^2 + (\omega + \epsilon - R)^2 - 2\Delta^{1/2} \\ &= 2\omega^2 + 2\epsilon^2 + 2\epsilon(Q - R) - 2\omega(Q + R) + (Q^2 + R^2) - 2\Delta^{1/2} \\ &= 2 \left[\epsilon^2 - \epsilon \left(\frac{NV^2}{\pi} \frac{B}{(\Delta_g^2 + B^2 - \omega^2)} \right) - (C^2 + \Delta^{1/2} - \omega^2) + \frac{N^2 V^4}{4\pi^2} \frac{B^2}{(\Delta_g^2 + B^2 - \omega^2)} \right], \end{aligned} \quad (5.27)$$

$$\text{where } C^2 = \frac{NV^2 \omega^2}{\pi(\Delta_g^2 + B^2 - \omega^2)} + \frac{N^2 V^4 \omega^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2}. \quad (5.28)$$

Now, consider the denominator of $G(\epsilon, \omega)$, that is

$$\begin{aligned} \text{Det } G^{-1} &= (\omega - \epsilon - \frac{V^2}{2\pi} M_{11})(\omega + \epsilon - \frac{V^2}{2\pi} M_{22}) - \frac{V^4}{4\pi^2} M_{21} M_{12} \\ &= (\omega - \epsilon - Q)(\omega + \epsilon - R) - \Delta^{1/2} \\ &= -\epsilon^2 - \epsilon(Q - R) + \omega^2 - \omega(Q + R) + QR - \Delta^{1/2} \\ &= -\epsilon^2 + \epsilon \left(\frac{NV^2}{\pi} \frac{B}{(\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta^{1/2} + C^2 - \omega^2) - \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2}. \end{aligned} \quad (5.29)$$

Hence, $\text{Tr} \left\{ \mathcal{T}_3 G(\epsilon, \omega) \mathcal{T}_3 G(\epsilon, \omega) \right\}$

$$= \frac{2 \left[\epsilon^2 - \epsilon \left(\frac{NV^2 B}{\pi (\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta'^2 + C^2 - \omega^2) + \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2} \right]}{-\epsilon^2 + \epsilon \left(\frac{NV^2 B}{\pi (\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta'^2 + C^2 - \omega^2) - \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2}} \quad (5.30)$$

The equation for poles is

$$-\epsilon^2 + \epsilon \left(\frac{NV^2 B}{\pi (\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta'^2 + C^2 - \omega^2) - \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2} = 0.$$

Let ϵ_1, ϵ_2 be the poles of $\text{Tr} \left\{ \mathcal{T}_3 G(\epsilon, \omega + i0^+) \mathcal{T}_3 G(\epsilon, \omega + i0^+) \right\}$,

and $\epsilon_1^*, \epsilon_2^*$ be the poles of $\text{Tr} \left\{ \mathcal{T}_3 G(\epsilon, \omega - i0^+) \mathcal{T}_3 G(\epsilon, \omega - i0^+) \right\}$.

Then these poles are

$$\epsilon_1 = \frac{NV^2 B}{2\pi (\Delta_g^2 + B^2 - \omega^2)} + i \sqrt{\Delta'^2 + C^2 - \omega^2} = \text{Re} \epsilon_1 + i \text{Im} \epsilon_1, \quad (5.31)$$

$$\epsilon_2 = \frac{NV^2 B}{2\pi (\Delta_g^2 + B^2 - \omega^2)} - i \sqrt{\Delta'^2 + C^2 - \omega^2} = \text{Re} \epsilon_1 - i \text{Im} \epsilon_1, \quad (5.32)$$

$$\epsilon_1^* = \frac{NV^2 B}{2\pi (\Delta_g^2 + B^2 - \omega^2)} + i \sqrt{(\Delta'^2 + C^2 - \omega^2)^*} = \text{Re} \epsilon_1^* + i \text{Im} \epsilon_1^*, \quad (5.33)$$

$$\epsilon_2^* = \frac{NV^2 B}{2\pi (\Delta_g^2 + B^2 - \omega^2)} - i \sqrt{(\Delta'^2 + C^2 - \omega^2)^*} = \text{Re} \epsilon_1^* - i \text{Im} \epsilon_1^*, \quad (5.34)$$



The integrals over ϵ of Eq. (5.23) that are then needed are

$$\begin{aligned}
 I_1 &= \int_{-\infty}^{\infty} d\epsilon \operatorname{Tr} [\mathcal{T}_3 G(\epsilon, \omega - i0^+) \mathcal{T}_3 G(\epsilon, \omega - i0^+)] \\
 &= 2 \int_{-\infty}^{\infty} d\epsilon \frac{\epsilon^2 - \epsilon \left(\frac{NV^2 B}{\pi (\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta^2 + C^2 - \omega^2) + \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2}}{(\epsilon - \epsilon_1^*)^2 (\epsilon - \epsilon_2^*)^2}. \quad (5.35)
 \end{aligned}$$

We choose ϵ_1^* to lie in the upper half-plane. Then by contour integration

$$I_1 = 2 \cdot 2\pi i \sum (\text{residue}) = 4\pi i \cdot 0 = 0. \quad (5.36)$$

The integral I_2 , on the other hand, is given by

$$\begin{aligned}
 I_2 &= \int_{-\infty}^{\infty} d\epsilon \operatorname{Tr} [\mathcal{T}_3 G(\epsilon, \omega - i0^+) \mathcal{T}_3 G(\epsilon, \omega + i0^+)] \\
 &= 2 \int_{-\infty}^{\infty} d\epsilon \frac{\epsilon^2 - \epsilon \left(\frac{NV^2 B}{\pi (\Delta_g^2 + B^2 - \omega^2)} \right) - (\Delta^2 + C^2 - \omega^2) + \frac{N^2 V^4 B^2}{4\pi^2 (\Delta_g^2 + B^2 - \omega^2)^2}}{(\epsilon - \epsilon_1)(\epsilon - \epsilon_2)(\epsilon - \epsilon_1^*)(\epsilon - \epsilon_2^*)}. \quad (5.37)
 \end{aligned}$$

Only ϵ_1 and ϵ_1^* are in the upper half-plane.

The residue of I_2 at ϵ_1 is

$$\begin{aligned}
 &\lim_{\epsilon \rightarrow \epsilon_1} \frac{(\epsilon - \epsilon_1) \cdot \text{numerator at } \epsilon = \epsilon_1}{(\epsilon - \epsilon_1)(\epsilon - \epsilon_2)(\epsilon - \epsilon_1^*)(\epsilon - \epsilon_2^*)} \\
 &= \frac{\text{numerator at } \epsilon = \epsilon_1}{(2i)^3 \operatorname{Im} \epsilon_1 (\operatorname{Im} \epsilon_1 - \operatorname{Im} \epsilon_1^*) (\operatorname{Im} \epsilon_1 + \operatorname{Im} \epsilon_1^*)}. \quad (5.38)
 \end{aligned}$$

The residue of I_2 at ϵ_1^* is

$$\begin{aligned} \lim_{\epsilon \rightarrow \epsilon_1^*} \frac{(\epsilon - \epsilon_1^*) \cdot \text{numerator at } \epsilon = \epsilon_1^*}{(\epsilon - \epsilon_1)(\epsilon - \epsilon_2)(\epsilon - \epsilon_1^*)(\epsilon - \epsilon_2^*)} \\ = \frac{-\text{numerator at } \epsilon = \epsilon_1^*}{(2i)^3 (\text{Im} \epsilon_1 - \text{Im} \epsilon_1^*) (\text{Im} \epsilon_1^* + \text{Im} \epsilon_1) \text{Im} \epsilon_1^*} \end{aligned} \quad (5.39)$$

Hence,

$$\begin{aligned} I_2 &= 2 \cdot 2\pi i \sum (\text{residue}) \\ &= 4\pi i \sum (\text{residue}) \\ &= \frac{4\pi i}{(2i)^3} \left[\frac{\text{numerator at } \epsilon = \epsilon_1}{\text{Im} \epsilon_1 (\text{Im} \epsilon_1 - \text{Im} \epsilon_1^*) (\text{Im} \epsilon_1 + \text{Im} \epsilon_1^*)} \right. \\ &\quad \left. - \frac{\text{numerator at } \epsilon = \epsilon_1^*}{\text{Im} \epsilon_1^* (\text{Im} \epsilon_1 - \text{Im} \epsilon_1^*) (\text{Im} \epsilon_1 + \text{Im} \epsilon_1^*)} \right] \\ &= 2\pi \frac{|\Delta'^2 + c^2 - \omega^2| + (\Delta'^2 + c^2 - \omega^2)}{(\text{Im} \epsilon_1 + \text{Im} \epsilon_1^*) \text{Im} \epsilon_1 \text{Im} \epsilon_1^*} \\ &= \frac{\pi}{\sqrt{\Delta'^2 + c^2 - \omega^2}} \cdot \frac{|\Delta'^2 + c^2 - \omega^2| + (\Delta'^2 + c^2 - \omega^2)}{|\Delta'^2 + c^2 - \omega^2|} \\ &= \frac{\pi}{\sqrt{\Delta'^2 + c^2 - \omega^2}} \cdot \left[1 + \frac{\Delta'^2 + c^2 - \omega^2}{|\Delta'^2 + c^2 - \omega^2|} \right] \end{aligned} \quad (5.40)$$

The thermal conductivity is, then

$$K = \frac{n}{8mk_B T^2} \int_0^{\infty} d\omega \frac{\omega^2 \operatorname{sech}^2(\frac{1}{2}\beta\omega)}{\sqrt{\Delta'^2 + C^2 - \omega^2}} \left(1 + \frac{\Delta'^2 + C^2 - \omega^2}{|\Delta'^2 + C^2 - \omega^2|} \right), \quad (5.41)$$

where n is the density of s-electrons.

V.5 Numerical Solution

Eq.(5.41) can be rewritten as

$$\frac{K}{n/mk_B} = \frac{1}{T^2} \int_0^{\infty} f(\omega) d\omega \left[1 + \frac{\Delta'^2 + C^2 - \omega^2}{|\Delta'^2 + C^2 - \omega^2|} \right], \quad (5.42)$$

where

$$f(\omega) = \frac{\omega^2 \operatorname{sech}^2(\frac{1}{2}\beta\omega)}{\sqrt{\Delta'^2 + C^2 - \omega^2}}. \quad (5.43)$$

We can see that the term $\left[1 + \frac{\Delta'^2 + C^2 - \omega^2}{|\Delta'^2 + C^2 - \omega^2|} \right]$ has two values depending on ω , that is 2 for $\omega < \sqrt{\Delta'^2 + C^2}$ and 0 for $\omega > \sqrt{\Delta'^2 + C^2}$. Hence, Eq.(5.42) becomes

$$\frac{K}{n/mk_B} = \frac{2}{T^2} \int_0^{\omega_0} f(\omega) d\omega, \quad (5.44)$$

where $\omega_0 = \sqrt{\Delta'^2 + C^2}$.

As the integral $\int_0^{\omega_0} f(\omega) d\omega$ cannot be solved analytically, its value has been computed numerically using Simpson's integration rule:

$$\int_0^{\omega_0} f(\omega) d\omega = \frac{\omega_0}{6} \left(\frac{3}{10} \right) \left[11f\left(\omega = \frac{\omega_0}{6}\right) - 14f\left(\omega = \frac{\omega_0}{3}\right) + 26f\left(\omega = \frac{\omega_0}{2}\right) - 14f\left(\omega = \frac{2\omega_0}{3}\right) + 11f\left(\omega = \frac{5\omega_0}{6}\right) \right]. \quad (5.45)$$

We must first calculate the value of ω_0 . The calculation has been done with the use of BCS expression for the energy gap:

$$\Delta_g = 3.1 k_B T_c \left(1 - \frac{T}{T_c} \right)^{1/2}. \quad (5.46)$$

The critical temperature T_c for Niobium is 9.5°K . Calculation has been done by taking units of energy in eV.

(27)

For weak-coupling limit V is small compare to E and U , so we can neglect the last term in B , i.e.,

$$B = E + U \langle n_\delta \rangle + \frac{2mP_0 V^2}{(2\pi)^3} \ln \left(\frac{\omega - \omega_D}{\omega + \omega_D} \right) \\ \approx E + U \langle n_\delta \rangle,$$

and since $E \sim -U/2$ (Niobium is nonmagnetic, $n_\uparrow = n_\downarrow = \frac{1}{2}$ or $\langle n_\delta \rangle = \frac{1}{2}$)

we can neglect the term B and we rewrite Δ'^2 and c^2 as

$$\Delta'^2 = \frac{N^2 V^4}{4\pi^2} \frac{\Delta_g^2}{(\Delta_g^2 - \omega^2)^2}, \quad (5.47)$$

$$c^2 = \frac{-NV^2 \omega^2}{\pi(\Delta_g^2 - \omega^2)} - \frac{N^2 V^4 \omega^2}{4\pi^2 (\Delta_g^2 - \omega^2)^2}. \quad (5.48)$$

Hence,

$$\Delta'^2 + c^2 = \frac{N^2 V^4 \Delta_g^2}{4\pi^2 (\Delta_g^2 - \omega^2)^2} - \frac{N^2 V^4 \omega^2}{4\pi^2 (\Delta_g^2 - \omega^2)^2} - \frac{NV^2 \omega^2}{\pi(\Delta_g^2 - \omega^2)} \\ = \frac{N^2 V^4}{4\pi^2 (\Delta_g^2 - \omega^2)} - \frac{NV^2 \omega^2}{\pi(\Delta_g^2 - \omega^2)},$$

and the value of ω_0 can be calculated by using the relation

$$\omega_0^2 = \Delta_g^2 + C^2, \text{ or by}$$

$$-\omega_0^2 + \frac{N^2 V^4}{4\pi^2(\Delta_g^2 - \omega^2)} - \frac{NV^2 \omega^2}{\pi(\Delta_g^2 - \omega^2)} = 0,$$

$$\omega_0^4 - \omega_0^2 \left(\Delta_g^2 + \frac{NV^2}{\pi} \right) + \frac{N^2 V^4}{4\pi^2} = 0,$$

which has the solution

$$\omega_0^2 = \left[\left(\Delta_g^2 + \frac{NV^2}{\pi} \right) + \sqrt{\left(\Delta_g^2 + \frac{NV^2}{\pi} \right)^2 - \frac{N^2 V^4}{\pi}} \right] / 2. \quad (5.49)$$

For niobium, we have taken $\frac{NV^2}{\pi} \approx 10^{-6}$ eV. This last numerical value has been determined in part by our treatment of the hybridization as a perturbation to the superconducting state. This implies that the hybridization term must be less than the superconducting gap. Otherwise the superconducting term must be treated as a perturbation of the hybridized states.

Since Δ_g is a function of temperature, ω_0 and $f(\omega)$ are also the functions of temperature. We use the temperature range 0.1-5.0°K. The temperature dependence of ω_0 , the integral $\int_0^{\omega_0} f(\omega) d\omega$ and the thermal conductivity are shown in the following tabulation and graph.

T (°K)	ω_0^2 ($\times 10^{-8} \text{ eV}^2$)	$\int_0^{\omega_0} f(\omega) d\omega$ ($\times 10^{-8} \text{ eV}^2$)	$k/\frac{n}{mk_B}$ [$\times 10^{-8} (\text{eV}/\text{°K})^2$]
0.1	733.779929	8.001357×10^{-22}	8.001357×10^{-20}
0.2	726.969427	2.134792×10^{-10}	5.336978×10^{-9}
0.3	720.158317	1.366207×10^{-6}	0.000015
0.4	713.346584	1.088014×10^{-4}	0.000068
0.5	706.534251	1.498380×10^{-3}	0.005994
0.8	686.093033	7.457881×10^{-2}	0.116529
1.0	672.462038	0.263333	0.263333
1.2	658.827953	0.580216	0.402928
1.4	645.190536	0.962750	0.491199
1.6	631.549693	1.331089	0.519957
1.8	617.905131	1.636953	0.505233
2.0	604.256524	1.882700	0.470675
2.4	576.946392	2.405690	0.417654
2.8	549.616564	3.477608	0.443573
2.9	542.780667	3.897193	0.463400
2.95	539.362182	4.134239	0.475063
3.0	535.943368	4.390246	0.487805
3.5	501.732335	8.067412	0.658564
4.0	467.474261	13.771323	0.860708
5.0	398.767035	29.648525	1.185941

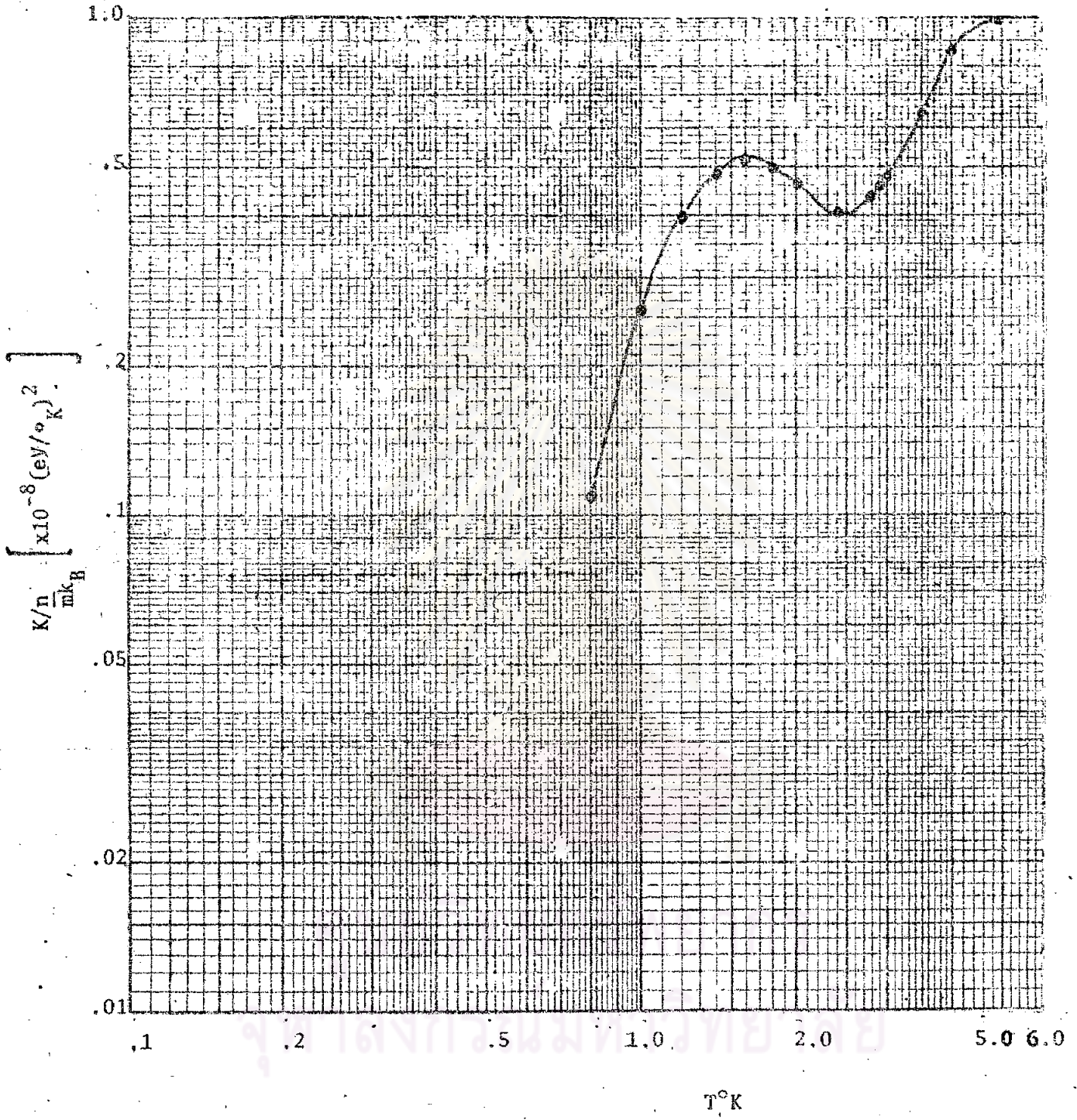


Fig. 5.1 Log-log plot of $K/(n/mk_B)$ vs temperature of Superconducting Nb

We can see from the graph that below T_c the thermal conductivity decreases according to the T dependence of electronic scattering of phonons. The minimum occurs at temperature about 2.4°K . After lowering further the temperature, the lattice conductivity increases while the electronic scattering of phonons decreases rapidly with the condensation of electrons into the superconducting ground state and the thermal conductivity starts to increase. The maximum of the thermal conductivity is at about 1.6°K . Below the maximum, the lattice conductivity is presumed to dominate, and the T^3 dependence is characteristic of boundary scattering. The data are in agreement with the work of Carlson and Satterthwaite.⁽²⁸⁾

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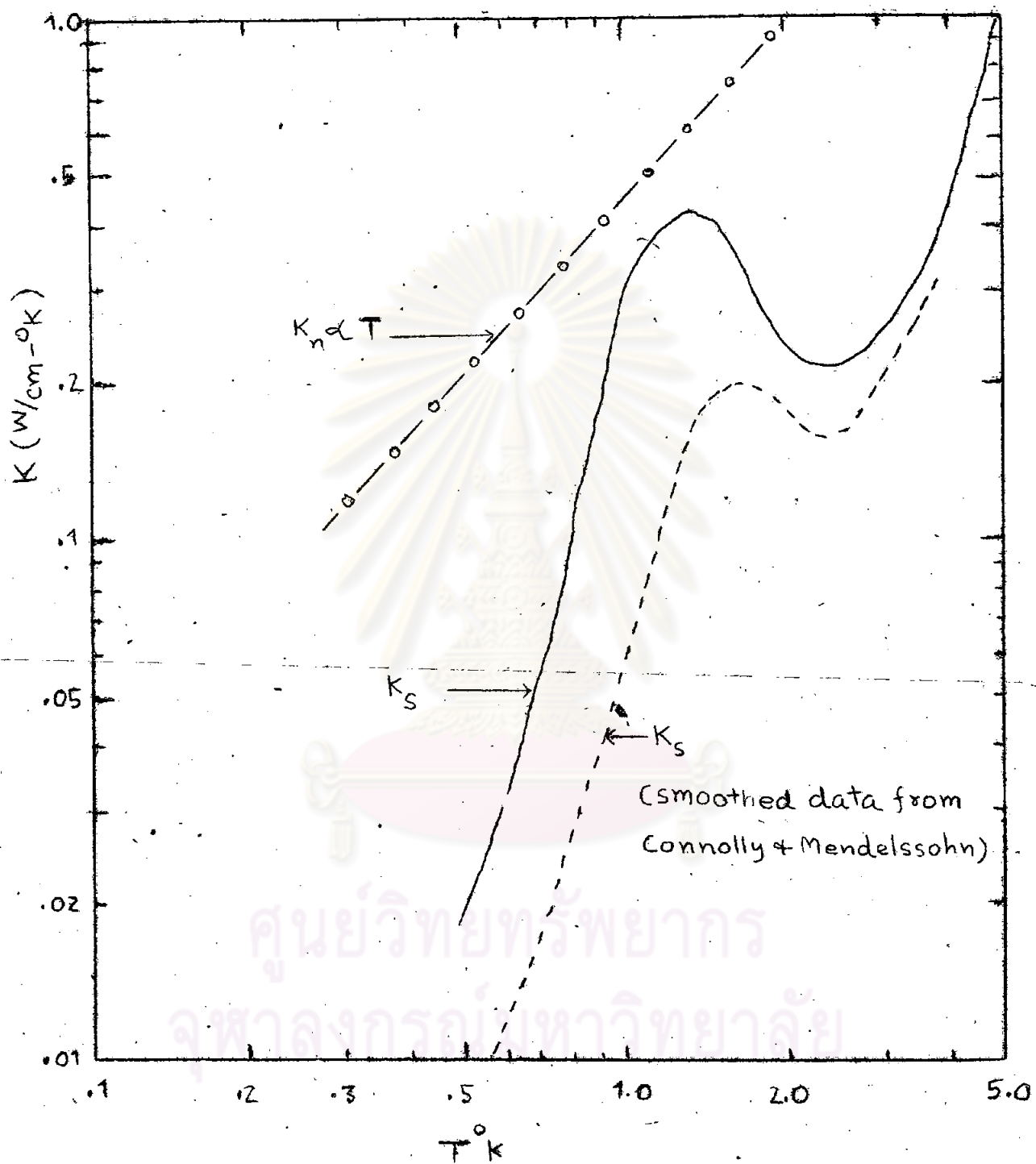


Fig.5.2 Thermal conductivity of normal and superconducting Nb.