PROXIMITY EFFECT AND THE THERMODYNAMIC PROPERTIES OF SUPERLATTICE SYSTEM

BY

JING WANG

A Thesis
Submitted to the Faculty of Graduate Studies
in Partial Fulfillment of the Requirements
for the Degree of

MASTER OF SCIENCE

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Abstract

A straightforward method, based on the self-consistent solution of the Bogoliubov equations using a step function approximation for the electron pair amplitude, is developed for the proximity effect of the superlattice system. The gap equation is obtained from the self- consistency condition imposed on the pair amplitude for various systems. Solving the thickness dependent gap function, the thermal properties of the systems can be determined. Comparison with other techniques that have been employed for the effect shows that the method is a reasonable theoretical treatment. The parameters of calculating the properties of these systems are within the standard BCS theory, and the results obtained in the analysis can be expressed in terms of certain universal relations which are independent of the particular material.

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Chapter 1

Introduction

In 1935, A. D. Misener [1] observed that the superconducting transition temperature of Pb films, which electroplated onto constantan wires, decreased below the bulk value with decreasing film thickness. In 1960, similar observations made on Sn films electroplated onto Au and Cu wires suggested that the lowering of the T_c was caused by the proximity or contact of a normal metal [2]. Since that time extensive investigations have been made on this so called *proximity effect* by using superimposed thin metal films. The studies have used a variety of analytical methods such as the measurement of T_c, H_c, persistent current, flux penetration and tunneling. After the experimental observations, several theoretical treatments of various aspects of the proximity effect were proposed, such as Cooper, de Gennes- Werthamer, and the McMillan tunneling model. There are also a number of works that have been done using the different approaches to investigate theoretically the properties of the proximity effect for superconducting thin films [3, 4, 5, 6, 7, 8, 9, 10, 11].

Theoretically, the proximity effect is believed due to the electron- electron interaction extending from the superconducting material into the normal conducting material. Therefore the theoretical treatment of the effect must be accounted for within the BCS theory. As we know, the BCS (Bardeen, Cooper, and Schrieffer) theory [12] is the standard theory of describing superconducting system. However, due to its non-linear nature, the BCS theory is difficult to solve for geometries other than the infinite homogeneous case. In this thesis, we will investigate a method of incorporating particular geometries other than the infinite homogeneous situation into the framework of the BCS theory.

For the system of a superconductor in contact with a normal metal, the so called SN structure, the major difficulty is to obtain a self- consistent expression for the spatially dependent electron pair amplitude. One extensively used and extremely useful technique to investigate the effect of the system is Ginzburg-Landau (GL) theory. The theory is based on the fact that the gap or order parameter approaches zero close to the transition point. The method can be used to investigate properties close to the critical point, like the critical temperature, as a function of film thickness [5, 6, 7].

However, if we are interested in properties away from the critical point the GL theory cannot be used, and we have to return to the original Bogoliubov equations. In such a situation, two general approaches can be used. One method is assuming that the pair amplitude has some convenient form, which is then used to solve the Bogoliubov equations. Properties of such system can be found in terms of the free parameters associated with the assumed pair amplitude. In order to have a straightforward solution, generally the assumed amplitude is an appropriate constant over the superconductor region, as this provides a relatively easy solution. Implicit in this approach is the condition that the assumed and the calculated amplitudes are close, so that the solution is "nearly self- consistent"[13, 14].

A more general technique which explicitly incorporates a self- consistency condition is a variational type of approach. The approach begins as before by assuming a particular form of the pair amplitude and solving the resultant equations. The free parameters associated with the assumed amplitude are then determined by a condition of the minimization of the free energy [15], or that the assumed and calculated pair amplitudes agree as closely as possible [14]. In both of these approaches it is possible to consider more general forms for the pair amplitude by employing a WKB type of expansion, which has the effect of reducing the Bogoliubov equations to a system of first order equations, these being relatively easier to solve.

Another method to solve the problem of such SN sandwich structure, somewhat different from the approaches we just discussed, is the McMillan tunneling model [16]. In this model a potential barrier is assumed to exist between the interface of the two joined metals, and tunneling through the barrier is treated by means of the transfer Hamiltonian method [17, 18]. The advantage of this model is that it is not restricted to the vicinity of the critical point. The relation between this approach and the wave function approach can be found in Refs. [19, 20, 21]. A brief discussion of this model will be presented in chapter 4.

In this thesis, we introduce a different method to study the proximity effect of superconducting thin films. The approach with regard to the self-consistency of the pair amplitude shares some of the characteristics of other approaches, but we use a self-consistency condition less stringent than demanding that the assumed and calculated pair amplitudes exactly coincide [22].

To start, we first work on the simplest geometry, a single film, and assume the pair amplitude is a constant in the superconductor region, so that we can construct explicit solutions to the Bogoliubov equation for the system. The requirement of the self-consistency condition is that the spatial average of the assumed and calculated order parameters be equal. Such a condition has been alluded to in previous works [13, 23], but does not appear to have fully exploited in calculating the properties of such a system away from the critical point. Naturally, this approximation is used in order to simplify some of the expressions. However, the approach provides a straightforward method to the single film system in finding both critical and noncritical properties with no parameters outside of those found in the BCS theory. We then apply the same method to the bilayer system incorporating Bloch's theorem. A final use of the approach is to a finite superlattice system. We find that the method gives reasonable results for certain ranges of the parameters, but breaks down outside those ranges. Many of the results obtained in this analysis can be expressed in terms of certain universal relations that are independent of the particular material.

The plan of the thesis is the following: In Chapter 1, we will briefly discuss the general properties of the superconductor. In Chapter 2, the BCS theory will be presented, and we briefly give a summary of the superconductor properties that can be obtained within the theory. In Chapter 3, in the first section we will discuss the property of the proximity effect, and in the following section we will introduce the major theoretical treatments on such effect. Starting from Chapter 4, we introduce a different approach to this effect for the simplest geometry. In the first section of the Chapter, we establish the energy eigenstates and give the general solution of the Bogoliubov equations, which will also be used in the infinite and the finite superlattice systems. We then use these solutions with the self- consistency condition to derive the gap equation. In the next section we solve the gap function and obtain the dependence of the critical temperature on the film thickness. In the last section of Chapter 5 we discuss the infinite superlattice by considering a finite alternating superlattice system with the limit $N \to \infty$, and then compare the results obtained with the infinite superlattice. In the last Chapter of the Thesis, we will investigate the properties of a finite superlattice system. In the first section of the Chapter, we set up the self-consistency gap function for the system. In the following section, we shall determine some critical properties of the system in term of the ratio of a/a_c and T/T_c, as well as the behaviour of the energy gaps. We then compare the results in certain limits with other approaches and discuss some of the problems which exist in the calculation. Finally we present some conclusions.

Chapter 2

Properties of Superconductors

As is well known, at sufficiently low temperature many metals and alloys undergo a phase transition to a *superconducting state.* In this state, the electric, magnetic and thermodynamic properties of the metal are radically different from its properties in the normal state. In this chapter, we will summarize these properties, since any theory of superconductivity must account for these properties.

1 Electrical Properties

The disappearance of electrical resistance of superconducting material at sufficiently low temperature is the major characteristic of superconductors. The earliest discovery of such behavior of the superconductor was H. K. Onnes in 1911, who found that mercury loses its resistance at 4.2 K. Since then others have confirmed the existence of other superconductors, and found that many metallic elements and alloys are superconductors as well.

The temperature at which the metal loses its resistance is called the *transi-*

tion temperature or *critical temperature*, normally denoted by T_c. For different superconducting materials the transition temperatures are different. These metals, which lose their resistance at the transition temperature, are said to pass into the *superconducting state*, and become superconductor. Since the transition is not accompanied by any structure and property change of the crystal lattice, it is interpreted as an electronic transition, in which the conducting electrons enter an ordered state.

In contrast, a material in the superconducting state is a truly perfect conductor. This implies the DC resistance of the superconductor is zero, and as a result, there is no DC power dissipation within the superconductor.

In 1913 Onnes also discovered that there was a "threshold value" of current density that can be carried by a superconductor before it reverts to its normal state. This is known as the *critical current density*, J_c, and he found that this quantity is a function of temperature; J_c increases as the temperature of the superconductor was lowered. The critical current is an important parameter in the description of superconductivity.

2 Magnetic Properties

Magnetic properties are an important and unique property of superconductors. The initial discovery was made by Meissner and Ochsenfeld in 1933, who found that *the magnetic flux is expelled from the interior of the superconductor and the magnetic induction* $\mathbf{B}$ *vanishes.* That is to say, inside a superconducting metal $\mathbf{B} = 0$, i.e., inside of a superconductor the flux density is not only constant, but the value of this constant is always zero! This important discovery is called the *Meissner effect.*

Since the Meissner effect was discovered, this unique property became one of the important tests of superconductivity, and any theory attempting to describe superconductivity must include this magnetic property in a fundamental way.

F. London and H. London suggested that the magnetic behavior of a superconducting metal might be correctly described by using the equation

$$\nabla \times \mathbf{J} = -\frac{ne^2}{m}\mathbf{B} \tag{2.1}$$

and

$$\frac{\partial \mathbf{J}}{\partial t} = \frac{ne^2}{m}\mathbf{E}, \tag{2.2}$$

which are known as the *London equations.* Equation (2.1) describes the resistanceless property of superconductor, as there is no electric field in a metal unless the current is changing; and Equation (2.2) describes the diamagnetism. The solution of the equations is

$$B_z(x) = B_z(0)e^{-x/\lambda_L^2}, \tag{2.3}$$

where λ_L is called the *London Penetration depth* and $\lambda_L^2 = m/\mu e^2$ The solution shows that the field decreases exponentially from the surface into the superconductor, and thus the field vanishes inside the superconductor, in accord with Meissner effect.

Due to the Meissner effect which says the total magnetic induction $\mathbf{B} = 0$ inside a superconductor, we establish

$$\mathbf{B} = \mathbf{H}_z(0) + \mu_0\mathbf{M} = 0, \tag{2.4}$$

where $\mathbf{H}_z(0)$ is the applied magnetic field, μ_0 is the permeability and $\mathbf{M}$ is the magnetization. Naturally, we get

$$\mathbf{H}_z(0) = -\mu_0\mathbf{M}.$$

This means the magnetization has the same magnitude but opposite direction to the applied field, and a cancellation is the result. The magnetic susceptibility, the ratio of magnetization to the applied field, must then be

$$\chi = -\frac{\mu_0 \mathbf{M}}{\mathbf{H}_z(0)} = -1.$$

Such a condition for the magnetization to cancel the external field exactly is referred to as *perfect diamagnetism.* Therefore, the superconductor is not only a perfect conductor but also a perfect diamagnet.

3 Thermodynamic Properties

During the transition from normal state to superconducting state, the thermal properties of the material are changed. This can be seen from the behavior of the specific heat.

3.1 Specific Heat

Experimental results show that the specific heat has a jump at the transition from the normal state to the superconducting state, i.e., the volue of specific heat at a superconducting state is greater than the volue at a normal state.

This can be seen by a derivation of the Gibbs free energy of the system:

$$G = U - TS + PV - \mathbf{H}_0 \cdot \mathrm{M},$$

and the first law of thermodynamics

$$dU = TdS - PdV + \mathbf{H}_0 \cdot d\mathrm{M},$$

where U is the internal energy, S is the entropy, P is the pressure, V is the volume, $\mathbf{H}_0$ is the applied field and $\mathbf{M}$ is the magnetization. At $T = T_C$

and $H_C = 0$, one can obtain the difference of the specific heat between the superconducting state and the normal state as

$$(C_S - C_N) = \frac{T_c}{\mu_0}(\frac{dH_c^2}{dT})^2_{T_C}. \quad (3.5)$$

This means in the absence of an applied field, and at the transition temperature, the specific heat of the superconducting state is greater than that of the normal state by an amount $\frac{T_c}{\mu_0}(\frac{dH_0}{dT})^2_{T_c}$.

The transition from normal to superconducting state is characterized by a continuous variation of both G and dG/dT. However, d^2G/dT^2 is discontinuous at T_c, leading to the jump in the heat capacity. Due to dG/dT being continuous at T_c, there is no latent heat associated with the transition between normal and superconducting state in a zero applied field. It is thus a *second- order phase transition.*

3.2 Energy Gap

Experiments at low temperatures also show that the specific heat of a superconductor in that region decreases exponentially as $T \rightarrow 0$. Such exponential behavior implies the existence of an energy gap, Δ_0, separating the normal states from the superconducting states. This gap leads to a small specific heat. The energy gap between the superconducting state and the normal state, lying just at the Fermi level, prevents the electron from being readily excitable. When the temperature is raised, the electrons are thermally excited across the gap and an amount of energy Δ_0 is absorbed for each of these electrons in the excitation process. When the temperature increases, and Δ_0 decreases, the gap vanishes at $T = T_c$. The width of the gap is of the order of k_BT_c.

From Boltzmann statistics, the number of electrons in the energy level above the gap is proportional to $e^{-\Delta_0/2k_BT}$ and the thermal energy absorbed in an excitation process is proportional to $\Delta_0 e^{-\Delta_0/2k_BT}$. Therefore, the specific heat is proportional to the derivative of the energy with a factor of temperature: $(1/T^2)e^{-\Delta_0/2k_BT}$. Since the T^2 term vanishes more slowly than the exponential term, the specific heat is nearly exponential:

$$C_S \propto \exp \frac{-\Delta_0}{2k_BT}.$$

Other experiment results, such as low temperature conductivity, the microwave absorption spectrum, etc., also confirm the existence of an energy gap in a superconductor.

4 Other Properties

We briefly state some other properties of superconductors.

4.1 Isotope Effect

In 1950, the study of different critical temperatures of various isotopes of the same element [24, 25] gave the result that the critical temperature for those isotopes is inversely proportional to the square root of the isotope's mass:

$$T_c \propto M^{-1/2}.$$

One conclusion from this observation is that the crystal lattice structure determines the properties of the electron found in those elemental isotopes.

This observation is called the *isotope effect*, and strongly supports the belief that the electron-phonon interaction is the origin of the superconductivity.

4.2 Two Types of Superconductors

It is known that magnetic fields can destroy superconductivity. The applied field at which the superconductor is destroyed is called the *critical field*, labeled by H_c; this transition is reversible. H_c is a temperature dependent function.

There are two types of superconductors that differ by their critical field. The first type is called a type I superconductor which only has one critical field H_c. Anther type is called a type II superconductor which has two critical fields, the lower one H_{c1} and the upper one H_{c2}. Both types of superconductor properties appear the same when $H < H_{c1}$, but in between H_{c1} and H_{c2} the type II superconductor is in a mixed state: the magnetic flux partially penetrates and forms small normal state cylinders. Above H_{c2} the type II superconductor becomes a normal metal.

The properties we discussed in this Chapter are just a brief summary of the experimental results. In the following Chapter, we will present the microscopic theory of superconductivity and also give the properties that can be obtained within the theory.

Chapter 3

BCS Theory

The modern theory of superconductivity was established by Bardeen, Cooper, and Schrieffer in their classic paper in 1957. The BCS theory, though approximate, provides a description of both thermal and dynamical properties of superconductors in the weak coupling limit. Generally the theory relies on three features of metallic solids: (1) the electron-lattice interaction; (2) the formation of an electron-pair bound state (the so called *Cooper pair state*) due to the coupling of the electrons to the lattice: and (3) the instability of the normal metallic state with respect to formation of a macroscopic condensed state of all pairs ($\mathbf{k}\uparrow$, $-\mathbf{k}\downarrow$) with antiparallel spins in momentum ($\mathbf{k}$) space. This condensed state exhibits the principal properties of superconductors, such as perfect diamagnetism, zero resistance, and so on. We will discuss these three features in this chapter.

1 The Attractive Interaction Between Two Electrons

In 1950, Fröhlich [26] suggested that an electron-electron attraction can be mediated by phonons, and that such an interaction is responsible for superconductivity. This electron-electron attractive interaction results from electron-lattice interactions. The interaction is treated to lowest order and the electron-electron correlations are decoupled in the mean field type approximation.

The electron-lattice interaction can be described by introducing phonons as quasiparticles representing vibrational models of the lattice. An electron moving in a solid and scattering on a lattice vibration absorbs or emits a phonon with energy $\hbar\omega_q$ and quasi momentum $\hbar\mathbf{q}$. If during this process the energy of incoming electrons (with energy $\varepsilon_{\mathbf{k}}$ and momentum $\hbar\mathbf{k}$) and scattered electrons (with energy $\varepsilon_{\mathbf{k}'}$) is conserved, then real scattering has taken place. Such events lead to the non-zero resistivity of metals at $T > 0$. For this process

$$\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} = \pm\hbar\omega_{\mathbf{q}},$$

where "-" corresponds to the emission and "+" to absorption of a phonon.

However, in the quantum mechanical description of scattering processes, there also exist virtual processes. Such processes involve the emission and subsequent reabsorption of a phonon in a short time interval. These virtual processes are composed of two parts: one describing phonon emission and the subsequent reabsorption process, and one describing the reverse process. Such processes can be described as follows: suppose that an electron with wave vector $\mathbf{k}_1$ emits a phonon $\mathbf{q}$, and the electron is scattered with a new wave vector $\mathbf{k}_1 - \mathbf{q}$. The emitted phonon is absorbed by another electron with wave vector $\mathbf{k_2}$, and after absorbing the phonon, the second electron has a new wave vector $\mathbf{k}_2 + \mathbf{q}$. The reverse process can be described by the first electron absorbing a phonon with wave vector -$\mathbf{q}$ and scatters from state $\mathbf{k}_1$ to state $\mathbf{k} - \mathbf{q}$; the second electron, after emitting a phonon -$\mathbf{q}$, changes from state $\mathbf{k}_2$ into state $\mathbf{k}_2 + \mathbf{q}$. According to second order perturbation theory the contribution of these two processes can be written as

$$< \mathbf{k}_1 - \mathbf{q}, \mathbf{k}_2 + \mathbf{q} \mid \mathbf{V}_1 \mid \mathbf{k}_1, \mathbf{k}_2 >= \frac{\mathbf{W}_{\mathbf{k}_1,\mathbf{k}-\mathbf{q}} \cdot \mathbf{W}^*_{\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}}}{\varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_1 - \mathbf{q}) - \hbar\omega_q}$$

and

$$< \mathbf{k}_1 - \mathbf{q}, \mathbf{k}_2 + \mathbf{q} \mid \mathbf{V}_2 \mid \mathbf{k}_1, \mathbf{k}_2 >= \frac{\mathbf{W}^*_{\mathbf{k}_1,\mathbf{k}_1-\mathbf{q}} \cdot \mathbf{W}_{\mathbf{k}_2,\mathbf{k}_2-\mathbf{k}_2+\mathbf{q}}}{\varepsilon(\mathbf{k}_2) - \varepsilon(\mathbf{k}_2 + \mathbf{q}) - \hbar\omega_{-q}},$$

where $\varepsilon(\mathbf{k}_1)$ and $\varepsilon(\mathbf{k}_1 - \mathbf{q})$ are the energies in state $\mathbf{k}_1$ and state $\mathbf{k}_1 - \mathbf{q}$, $\varepsilon(\mathbf{k}_2)$ and $\varepsilon(\mathbf{k}_2 + \mathbf{q})$ are the energies in state $\mathbf{k}_2$ and $\mathbf{k}_2 + \mathbf{q}$, the $\mathbf{W}$ terms are the electron-phonon interaction matrix elements, $\mathbf{W}_{\mathbf{k}_1,\mathbf{k}_1-\mathbf{q}}$ is the interaction between the first electron and phonon, and $\mathbf{W}_{\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}}$ is the interaction between the second electron and phonon. Conservation of energy requires that

$$\varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_1 - \mathbf{q}) = \varepsilon(\mathbf{k}_2) - \varepsilon(\mathbf{k}_2 + \mathbf{q}),$$

and for the electron-phonon matrix elements

$$\mathbf{W}_{\mathbf{k}_1,\mathbf{k}_1-\mathbf{q}} = \mathbf{W}_{\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}}.$$

The total contribution of these two processes to the energy is then

$$\mathbf{V}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} =\mid W_{\mathbf{k}_1,\mathbf{k}_1-\mathbf{q}} \mid^2 \frac{\hbar\omega_{\mathbf{q}}}{[\varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_1 - \mathbf{q})]^2 - (\hbar\omega_q)^2}. \tag{1.1}$$

One notices that if $\mid \varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_1 - \mathbf{q}) \mid < \hbar\omega_q$ in the above equation, then $\mathbf{V}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} < 0$; that is, the interaction is attractive. This means only the electrons within a $\pm\hbar\omega_q$ band measured at Fermi surface have this attractive interaction. These states in the Fermi sea are fully occupied and cannot interact with other electrons in the neighboring energy levels. If this attraction overcomes the Coulomb repulsion between electrons, this leads to a net attraction between the electrons in that region. Such a net attractive interaction results in a stable superconducting state.

2 Cooper Pairs State

Following Fröhlich's discovery, Cooper[27] showed that if the attractive potential in Equation (2.1) is approximated by a negative constant, -V, in the energy interval $\hbar\omega_D$ above ε_F, then such a potential introduces a binding between these two electrons.

When two electrons are added to a electron gas at $T = 0$, they must occupy the state above the Fermi level because of the Pauli exclusion principle. For the particular situation of an electron pair of zero total momentum and in its singlet spin (s=0) state, the Schrödinger equation for the eigenvalues, E, and eigenfunction,Ψ, of such an electron pair can be reduced to

$$(H_0 + H_1)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}),$$

where $H_0 = -\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator of the pair, H_1 is the two-body interaction, and $\mathbf{r}$ is the relative position of the pair. Now let us make an expansion of Ψ in a plane wave pair state,

$$\Psi = \sum_i a_i \phi_i(\mathbf{r}),$$

where $\phi_i(\mathbf{r}) = \exp(i\mathbf{k}_i \cdot \mathbf{r})$ Then

$$H_0\phi_i(\mathbf{r}) = \frac{\hbar^2 k_i^2}{m}\phi_i(\mathbf{r}).$$

The pair must be in the respective state $\mathbf{k}_i \uparrow$, $\mathbf{k}_i \downarrow$, so that the total momentum is zero, and the net spin, $\uparrow$ or $\downarrow$, of the pair is also zero.

Substituting Ψ into the Schrödinger equation, and multiplying by $\phi_j^*(\mathbf{r}) = \exp[-i\mathbf{k}_j \cdot \mathbf{r}]$ and integrating over all space we can find

$$\sum_i [(\frac{\hbar^2 k_j^2}{m} - E)\delta_{i,j} + < j \mid H_1 \mid i >] a_i = 0, \qquad (2.2)$$

where

$$< j \mid H_1 \mid i >= \int d\mathbf{r} \phi_j^*(\mathbf{r}) H_1(\mathbf{r}) \phi_i(\mathbf{r}).$$

If

$$< j \mid H_1 \mid i >= \begin{cases} -V & \text{if } \varepsilon_F \le \varepsilon \le (\varepsilon_F + \hbar\omega_D) \\ 0 & \text{otherwise} \end{cases},$$

from Equation (2.2) we get

$$a_j = \frac{VC}{2\varepsilon_j - E},$$

where $\varepsilon_j = \frac{\hbar^2 k_j^2}{2m}$, and

$$C = \sum_i a_i = N(0) \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} a(\varepsilon) d\varepsilon$$

and $N(0)$ is the density of state at the Fermi surface. Now, the consistency condition yields the eigenvalue equation

$$1 = N(0)V \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{d\varepsilon}{2\varepsilon - E}.$$

For $E < 2\varepsilon_F$ the solution is

$$E - 2\varepsilon_F = -2\hbar\omega_D [\exp(\frac{2}{N(0)V}) - 1]^{-1}.$$

Therefore the potential $-V$ introduces a binding between these two electrons with binding energy

$$\Delta \cong -2\hbar\omega_D \exp[\frac{-1}{N(0)V}]. \qquad (2.3)$$

In this expression $\hbar\omega_D$ represents an average phonon energy. The bound state represented by the above equation has the following important features:

(1) Since the binding energy has its largest value for the state of the pair at rest, (that is, the total pair momentum $\mathbf{k}_1 + \mathbf{k}_2 = 0$), Δ represents the binding energy of the pair $\mathbf{k}$ and -$\mathbf{k}$.

(2)The spin of pair is compensated: a singlet state is produced.

(3)The bound state has a lower energy than a pair of free electrons at the Fermi level, and therefore the electron gas state is unstable against such electron pair formation. The size of the two electrons is

$$\xi_0 \approx \frac{\hbar v_F}{k_b T_c} \sim 10^4 \mathring{A},$$

where v_F is Fermi velocity for electrons, and ξ_0 is defined as the *coherence length.*

A system of such pairs may condense into a superfluid state if the attraction is stronger than the Coulomb repulsion between electrons.

Furthermore, if Δ is of the order of $k_B T_c$, Equation (2.3) can be written in terms of T_c in the weak coupling limit $N(0)V \ll 1$ as

$$T_c = \theta_D \exp[\frac{-1}{N(0)V}],$$

where $k_B\theta_D = \hbar\omega_D$, θ_D is the *Debye temperature* and ω_D is called the *Debye frequency.* This is used to estimate the parameters of the microscopic theory in terms of the single Cooper pair state.

3 Superconducting Ground State

For a system of Cooper pairs, the wave functions of different pairs overlap appreciably, forming a condensed and coherent state of pairs in the superconducting phase: this state is called the *superconducting ground state.* Since ψ is made up of states of electrons being excited above the normal ground state by a wave number of order Δk, $\Delta k \sim 1/\xi_0 \sim 10^{-4}k_F$, according to the Pauli exclusion principle that electron can only be excited into those unoccupied states, and therefore only electronic states within a wave number range $10^{-4}k_F$ of the Fermi surface are involved in the superconducting phase transition.

The Hamiltonian of the ground state of many Cooper pairs in the BCS model is

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}'\mathbf{k}} c^{+}_{\mathbf{k}'\uparrow} c^{+}_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}. \tag{3.4}$$

The first term describes the single electron energy ε_k , and $n_{\mathbf{k}}\sigma = c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$, the number of electrons in state $\mid \mathbf{k}\sigma >$. The second term describes the pairing part for the system of pairs scattering from the state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ into state $(\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$.

In order to determine the eigenenergies of the Hamiltonian, we can use either Schrieffer's variational method [28] or the transformation method developed by Bogoliubov and Valatin [29]. Here we briefly discuss the variational calculation. Since in the superconducting ground state we only consider the pair state, in Equation (3.4) only that term that connects pairs with zero net momentum is used:

$$\mathcal{H} = \sum_{\mathbf{k}} 2\varepsilon_{\mathbf{k}} b^{+}_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} b'^{+}_{\mathbf{k}} b_{\mathbf{k}},$$

where $b^{+}_{\mathbf{k}} = c^{+}_{\mathbf{k}\uparrow} c^{+}_{-\mathbf{k}\downarrow}$ and $b_{\mathbf{k}} = c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}$ are the creation, and the annihilation operator for the pair in $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$.

In the ground state, Schrieffer's wave function is

$$\mid \psi_0 >= \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} b^{+}_{\mathbf{k}}) \mid 0 >,$$

where $| \; 0 >$ is ground state (vacuum state), and $v_{\mathbf{k}}$, $u_{\mathbf{k}}$ are the probabilities of finding a Cooper pair in an occupied state and an empty state. The normalization condition requires that

$$v_{\mathbf{k}}^2 + u_{\mathbf{k}}^2 = 1.$$

To find the expectation value, we introduce a term $-\mu O_N$, where μ is the chemical potential and O_N is the electron number operator. We have

$$< 0 \mid \mathcal{H} - \mu O_N \mid >= 2\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - \mu)v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}.$$

For convenience, let us define $u_{\mathbf{k}} = \sin\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$. We then minimize the expectation value

$$\frac{d}{d\theta} < 0 \mid \mathcal{H} - \mu O_N) \mid 0 >= 0$$

and obtain

$$2(\varepsilon_{\mathbf{k}} - \mu)\sin 2\theta_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \cos 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} = 0.$$

From this equation we can find

$$v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2 = -\frac{\varepsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}},$$

which results in:

$$v_{\mathbf{k}}^2 = 1/2[1 - \frac{(\varepsilon_{\mathbf{k}} - \mu)}{E_{\mathbf{k}}}]$$

and

$$E_{\mathbf{k}} = [(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2]^{1/2}. \tag{3.5}$$

In this equation, $| \; \Delta_{\mathbf{k}} \; |$ is the superconducting gap that is determined from the self-consistent equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh(\frac{\beta E_{\mathbf{k}}}{2}). \tag{3.6}$$

If $V_{\mathbf{k}\mathbf{k}'}$ is approximated by a negative constant, then $\Delta_{\mathbf{k}} = \Delta$, and

$$\Delta = \hbar\omega_D \exp[\frac{-1}{N(0)V}],$$

and so Equation (3.6) yields a solution of either $\Delta \equiv 0$ or $\Delta \neq 0$. For $\Delta \neq 0$ we have the gap equation

$$1 = \frac{V}{N(0)} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} \tanh(\frac{\beta E_{\mathbf{k}}}{2}), \tag{3.7}$$

where

$$E_{\mathbf{k}} = [(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta^2]^{1/2}$$

Equations (3.6) and (3.7) constitute the simplest BCS solution for an isotropic gap. One we can see that $E_{\mathbf{k}}$ is always nonvanishing and reaches a minimum $E_{\mathbf{k}} = \Delta$ for electrons placed on the Fermi surface, when $\varepsilon_{\mathbf{k}} = \mu$. Therefore the meaning of the gap can be understood: it is the gap for single electron excitations from the superconducting (condensed) state to a free electron state. The thermally excited electrons across the gap do not introduce nonzero resistivity because their contribution is short– circuited by the presence of the gap condensate that carries a current with no resistance. The same holds true even for the superconducting system for which the gap vanishes in some direction of $\mathbf{k}$ space.

All thermodynamic properties are associated with thermal excitations; the energies that are specified by Equation (3.5) contain $\mid \Delta_{\mathbf{k}} \mid$ or Δ as a parameter to be determined self-consistently from Equation (3.6) or (3.7).

4 Summary of The Properties

In this section, we will briefly summarize the results that may be obtained within the BCS theory.

(1). At $T = 0$, Equation (3.7) reduces to

$$1 = [V/2N(0)] \sum_{\mathbf{k}} E_{\mathbf{k}}^{-1},$$

and the value $\Delta = \Delta_0$ at $T = 0$ for $N(0)V \ll 1$ is given by

$$\Delta_0 = \frac{\hbar\omega_D}{\sinh[1/N(0)V]} \approx 2\hbar\omega_D \exp[-\frac{1}{N(0)V}]. \tag{4.8}$$

One notes a striking similarity between Equation (4.8) and (2.3) for $N(0)V \ll 1$, which represents the weak coupling limit.

(2). If we choose the origin of energy at μ, then Equation (3.7) can be written in the integral form

$$1 = V \int_0^{\hbar\omega_D} \frac{N(\varepsilon)d\varepsilon}{(\varepsilon^2 + \Delta^2)^{1/2}} \tanh[\beta/2(\varepsilon^2 + \Delta^2)^{1/2}]. \tag{4.9}$$

Since $\hbar\omega_D \ll \mu$, we can substitute $N(\varepsilon) \approx N(\varepsilon_F) = N(0)$ within the integration range. This allows an evaluation of the critical temperature for which $\Delta = 0$:

$$T_c = 1.14\theta_D \exp[-\frac{1}{N(0)V}]. \tag{4.10}$$

From this equation we see that because of exponential factor the critical temperature T_c is much smaller than the Debye temperature.

(3). Solving Equations (4.8) and (4.10), we obtain the ratio

$$\frac{2\Delta_0}{k_B T_c} \approx 3.53, \tag{4.11}$$

which is used frequently to test the applicability of the BCS model. This ratio also can be obtained in the strong coupling limit [30].

(4). The energy $E_{\mathbf{k}}$ represents electronic excitations across the energy gap. The entropy of a superconductor can be written as

$$S = -2k_B \sum_{\mathbf{k}} [f_{\mathbf{k}} \ln f_{\mathbf{k}} + (1 - f_{\mathbf{k}}) \ln(1 - f_{\mathbf{k}})], \tag{4.12}$$

where $f_{\mathbf{k}} = f(E_{\mathbf{k}}) = [1 + \exp(\beta E_{\mathbf{k}})]$ is the Fermi-Dirac distribution function. Therefore the free energy of superconducting state is

$$F_S = 2\sum_{\mathbf{k}} E_{\mathbf{k}} f_{\mathbf{k}} - TS. \tag{4.13}$$

We should note that the thermodynamic properties are determined only if the chemical potential $\mu = \mu(T)$ and the energy gap $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}(T)$ are explicitly found, since only the spectrum of single electron excitations, characterized by the energies $E_{\mathbf{k}}$, are uniquely determined. $\Delta(T)$ is determined from Equation (4.9) and the chemical potential is determined from the conservation of number of electrons, N_e, i.e. from the condition $\sum_{\mathbf{k}} f_{\mathbf{k}} = N_e$.

(5). The difference $F_S - F_N$ between the free energies in the superconducting phase F_S and normal phase F_N can be equated to the magnetic free energy by $F_S - F_N = \frac{H_c^2 V}{8\pi}$, where V is the volume of the system. We then obtain the approximate relation:

$$\frac{H_c(T)}{H_c(0)} \approx 1 - (\frac{T}{T_c})^2, \tag{4.14}$$

where H_c is the thermodynamic critical field. For an applied field $H > H_c$, superconductivity is destroyed because the spin singlet bound state is destroyed by the thermal fluctuations. The pair binding energy is then effectively overcome by the magnetic energy, so that the pairs break up into single electrons. This type of behavior characterizes type I superconductors.

(6). From the calculation of the specific heat, we can obtain a discontinuity of the form, at $T = T_c$,

$$\frac{C_S - C_N}{C_N} \approx 1.43. \tag{4.15}$$

At low temperature, the specific heat decreases exponentially

$$C_S \sim \exp[\frac{\Delta_0}{k_B T}], \tag{4.16}$$

for the case of an isotropic gap. If the gap is anisotropic : $\Delta = \Delta_{\mathrm{k}}(T)$, then the low temperature dependence of the specific heat does not follow Equation (4.16) but rather a T^n power law, with n depending on the gap of anisotropy. The specific heat grows with T because the number of thermally broken pairs increases with rising temperature; at $T = T_c$ ($k_B T_c = \Delta_0$), all bound pairs dissociate thermally at which point C_S reaches a maximum. If the temperature is raised above T_c, the excess specific heat drop rapidly to zero since no pairs are left to absorb the energy. This type of behavior is observed in a superconductor with an isotropic gap.

(7). The spin part of the static magnetic susceptibility vanishes as $T \longrightarrow 0$. This can be explained as the direct consequence of the binding of electrons in the condensed state into singlet pairs. Therefore the Meissner effect is present at $T = 0$ because of the orbital part of the susceptibility. The temperature dependence of the penetration depth is given by

$$\frac{\lambda(T)}{\lambda(0)} = [\frac{\Delta(T)\tanh(\Delta/2k_B T)}{\Delta_0}] \approx [1 - (\frac{T}{T_c})^4]^{1/2}. \qquad (4.17)$$

This result is obtained under the assumption that the coherence length $\xi \simeq \hbar V_F/\Delta$ is much larger than λ.

(8). The relative ratio $\kappa = \lambda/\xi$ determines the type of superconductivity behavior in a magnetic field. From $\xi \sim \Delta^{-1}$, we can get, as $T \rightarrow T_c$, $\xi \sim (T_c - T)^{-1/2}$. The same dependence for $\lambda(T)$ can be obtained from Equation (4.7) as $T \longrightarrow T_c$. From the Ginzburg-Landau theory, one can show that if $\kappa \leq 1/\sqrt{2}$, the superconductivity is of the first kind; if $\kappa \geq 1/\sqrt{2}$, then it is of the second kind. The κ is directly related to the penetration depth $\lambda(T)$. Equation (4.14), the thermodynamic critical magnetic field, has the form

$$H_c(T) = \Phi_0 \frac{\sqrt{2}}{\kappa\lambda^2(T)}$$

or

$$H_c(T) = \frac{\Phi_0}{2\pi\sqrt{2}\xi(T)\lambda(T)}, \tag{4.18}$$

where $\Phi_0 = \hbar c/2e$ is the magnetic-flux quantum. This value of the field terminates superconductivity of the first kind. For superconductivity of the second kind, the corresponding field equation is

$$H_{c2} = \kappa\sqrt{2}H_c = \frac{\Phi_0}{2\pi\xi(T)^2}. \tag{4.19}$$

For the fields $H_{c1} < H_0 < H_{c2}$, with $H_{c1} = H_c(0)\ln[\kappa/\sqrt{2\kappa}]$, the superconducting phase is inhomogeneous, composed of a lattice of vortices, each of the form of a tube containing one flux quantum, penetrating the sample. The high-T_c superconductors are all superconductors of the second kind.

Chapter 4

Proximity Effect of Superconducting Thin Films

In this chapter, we shall briefly discuss the basic properties of the proximity effect and introduce several major theoretical models of the effect.

Cooper, in 1961 [3], introduced a physical argument of the proximity effect, which can be described as follows. In the BCS theory the range between the attractive electrons is very short ($\sim 10^{-4} \mathring{A}$); however, the size of the wave packet or the correlation distance of the attractively bound Cooper pairs is of the order of the coherence length. Due to this longer coherence length, the Cooper pairs can extend a considerable distance into a region in which the interaction between electrons is not attractive. Therefore, if a thin normal metal layer N is deposited onto a superconducting metal S, and if the electrical contact between the two is good, the Cooper pairs can leak into the normal layer. As a result, the ground state energy of this thin bimetallic layer is characterized by some average of the interaction parameter $N(0)V$ over both metals, which in turn determines the energy gap of the layer and its transition temperature. From such an argument, one can understand that the proximity effect should yield information on the electron- electron interaction in the normal metal.

1 Properties of the Proximity Effect

Experimental results of the contact between two layers show that the critical properties of the superconducting thin film are different from the bulk superconductor. One important facet of the proximity effect is that it must depend on the nature of the boundary between the two metals and on the relative thickness of the two layers: the thicker the normal layer, the smaller the average interaction and the smaller the influence on the properties of the superconducting film. The properties of the effect generally can be summarized as follows:

(1). The critical thickness, which is always smaller than the coherence length of the bulk superconductor, decreases with a decrease of the effective mean free path. The deposited films have a very short electron mean free path in the normal state and their coherence length is modified.

For a SN sandwich structure, the transition temperature, T_s, is lower that in the bulk superconductor materials. An empirical relation was suggested:

$$(\frac{T_s}{T_c})^2 = 1 - \frac{1}{0.2 + 0.8R_s},$$

where T_s is the transition temperature of the system, T_c is the bulk transition, $R_s = a/a_c$ is the ratio of the thickness of the superconducting film, and a_c is critical thickness below which no superconductivity is observed for a constant thickness of the normal metal film. This relation gives a general picture of the reduced transition temperature.

(2). The magnetic aspect of the proximity effect is that a magnetic or nonmagnetic metal in contact with a superconductor breaks Cooper pairs and hence suppresses superconductivity. This process is equivalent to paramagnetic impurities or a critical current in a superconductor. If the normal metal is magnetic, it should have a more pronounced effect because of the additional interaction of spins with the conduction electrons.

(3). The study of superimposed films Ag/Pb showed the existence of persistent currents through the couple. Such a study also shows that the induced gap in the normal metal is much smaller than that of pure superconductor's value [31]. An exponentially decreasing energy gap with increasing normal Ag film thickness is also found. The gap was found to be insensitive to temperature far below the T_c of the pure Pb superconductor [32], which is consistent with the proximity mechanism of de Gennes. The gap was independent of the applied longitudinal field up to a certain value above which it decreased linearly.

(4). The critical field study of double films, due to Duffy and Meissner [33], established that the proximity effect could be explained by assuming a modified mean free path for the couple and a total film thickness which corresponds to that of the superconducting film only.

If both metal films are superconductors of different T_c's, the T_c of the couple varies from one extreme to another as the relative thickness of the two films is varied [34, 35]. Such a behavior is intuitively expected and is illustrated by the data on Pb/Al film couples. The quantitative results are in good agreement with the de Gennes theory applicable to such a case.

In the following section, we will review the major theoretical treatments.

2 Theoretical Methods

Based on the experimental results of the layered structure of superconducting materials and the related boundary problems, several theoretical treatments have been proposed. In this section we briefly review these major treatments.

2.1 Cooper Model

The model is based on a modification of parameter $[N(0)V]$ which occurs in BCS expression for the energy gap

$$\Delta_0 = 2(\hbar\omega)_{av} \exp[-1/N(0)V]. \tag{2.1}$$

The system considered is that of two thin metallic films in contact over the plane $x = 0$. One side is a superconductor with thickness D_S and the other side is a normal metal with thickness D_N. The electron-electron interaction is then a function of momentum, relative coordinate r and the absolute position of the two electrons in the x direction, x_1 and x_2:

$$V(r, k, ...) = \begin{cases} V & \text{if } x_1 < 0 \text{ and } x_2 < 0 \\ 0 & \text{if } x_1 > 0 \text{ or } x_2 > 0 \end{cases} \tag{2.2}$$

Due to the electron-electron interaction there is a nonzero matrix element $V_{k,k'}$ for scattering from a two-electron state k to k'. This element, summed over all k' and averaged over k in the interaction region, yields $[N(0)V]_{av}$ in (2.1), which determines the energy gap and the transition temperature. This average will be increased if the electron normalization volume is increased while the electron-electron interaction acts over only a part of the volume. This results in a decrease of the transition temperature of the superconductor in contact with a normal metal. The same argument implies that for a normal metal in contact with a superconductor, the normal metal can become a superconductor[3].

A simple case is two metals in perfect contact with the same Fermi energy and the same effective mass, with $[N(0)V]$ in the normal metal being zero and D_S and D_N much less than the coherence length ξ. In such a situation, we have:

$$[N(0)V]_{eff} = \frac{D_S}{D_S + D_N}[N(0)V]_S, \tag{2.3}$$

where $[N(0)V]_S$ is the interaction constant for a superconductor and $[N(0)V]_{eff}$ is that for the two films in contact. The limit $D_S, D_N \ll \xi$ is called the *Cooper limit.* Due to the exponential dependence of the energy gap on $N(0)V$, under the above conditions even the thinnest films of a normal metal would produce a drastic alteration of the energy gap in a thin superconducting film. The transition temperature T_c for the film complex can be obtained from

$$T_c = 1.14\theta_D \exp\{-[N(0)V]^{-1}_{eff}\}, \tag{2.4}$$

where θ_D is Debye temperature.

However, in an experimental condition, there always exists a barrier between the contact metals, which will tend to separate the two materials. The causes could be an oxygen layer or any mechanical barrier or separation. Therefore, the actual reduction factor would have the form:

$$\frac{D_S}{D_S + \beta D_N}, \tag{2.5}$$

with $0 \geq \beta \leq 1$ and β is a parameter characterizing the barrier between the films.

The effective penetration of electrons from one region to another is limited among other things by the electron mean free path; the further the superconducting electrons penetrate into the normal area the smaller the energy gap will be.

2.2 De Gennes-Werthamer Model

The assumption for the system is that the electrons are coupled by a point interaction $-V(\mathbf{r}_i)\delta(\mathbf{r}_i - \mathbf{r}_j)$. The $V(\mathbf{r})$ are not the same in the N and S regions. In the S regions, $V = V_S$ is positive and attractive. In the N regions, $V = V_N$ may be of either sign, depending on a delicate balance between the Coulomb repulsion and the phonon-induced attraction.

To derive the Fermi-type excitations, the one-electron operator $\psi_\alpha^\dagger(\mathbf{r})$ can be written:

$$i\frac{\partial \psi_\alpha^\dagger}{\partial t}(r) = [\frac{p^2}{2m} + U(r)]\psi_\alpha(r) - V(r) \times \sum_\beta \psi_\alpha^\dagger(r)\psi_\beta^\dagger(r)\psi_\beta(r). \qquad (2.6)$$

Here, α and β are spin indices; the origin of energies is at the Fermi level, and U is the one electron potential with different values in both metals which also includes the effect of impurities and boundaries. The linearization of the last term of (2.6) is

$$V_n \psi_\alpha^\dagger(r)\psi_\beta^\dagger(r)\psi_\beta(r) \rightarrow V_n \langle \psi_\alpha^\dagger(r)\psi_\beta^\dagger(r)\rangle \psi_\beta(r). \qquad (2.7)$$

The bracket denotes a thermal average. The only non-vanishing terms in (2.7) come from

$$V(\mathbf{r})\langle \psi_\downarrow^\dagger(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{r})\rangle = -V(\mathbf{r})\langle \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\rangle = \Delta^\dagger(\mathbf{r}), \qquad (2.8)$$

where $\Delta(\mathbf{r})$ is called the pair potential. We now look for eigenmodes of the linearized equation of the form

$$\psi_\uparrow(\mathbf{r}t)[u_n(r)e^{-iE_nt}\gamma_{n\uparrow} + v_n^\dagger(r)e^{iE_nt}\gamma_{n\downarrow}], \qquad (2.9a)$$

$$\psi_\downarrow(\mathbf{r}t) = \sum_n [u_n(r)e^{-iE_nt}\gamma_{n\downarrow} - v_n^\dagger(r)e^{iE_nt}\gamma_{n\uparrow}], \quad (2.9b)$$

where $\gamma_n^\dagger \mu \gamma_n \mu$ are new fermion operators $[\gamma_{n\mu}^\dagger \gamma_{m\sigma}] = \delta_{nm}\delta_{\mu\sigma}$ and the excitation energy E_n is restricted to positive values. u and v are the eigenfunctions of the following system of equations:

$$Eu = [(1/2m)p^2 + U(r)]u + \Delta v, \quad (2.10a)$$

$$Ev = -[(1/2m)p^2 + u(r)]v + \Delta^\dagger u. \quad (2.10b)$$

To solve for the u's and v's, we must write down the self- consistency requirement obtained from Equations (2.8) and (2.9). Due to the Fermi function $f(E_n) = 1/[1 + \exp(E_n/T)]$, the average in (2.8) gives

$$\Delta(\mathbf{r}) = V(\mathbf{r})\langle\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle = V(r) \times \sum_n v_n^\dagger(\mathbf{r})u_n(\mathbf{r})[1 - 2f(E_n)]. \quad (2.11)$$

To ensure the convergence of this equation, we cut off the interaction V when the excitation energy ϵ_n is higher than ω_D, the local Debye frequency, in agreement with the original BCS procedure.

The pair potential $\Delta(r)$ will be spatially dependent for these systems. This dependence has a important consequence: the eigenfunctions $u_n(\mathbf{r})$, $v_n(\mathbf{r})$ of Equation (2.10) are not simply proportional to the one electron wave function in the normal state w_n, i.e., the electron pairing is not obtained by pairing one electron in a state w_n and another in the time- reversed state w_n, which only holds when $\Delta(\mathbf{r})$ may be taken as independent of r, as in an infinite, pure metal or homogeneous alloy.

The pair potential $\Delta(\mathbf{r})$ is a natural "order parameter" for the inhomogeneous systems. We use the "condensation amplitude" $F(\mathbf{r})$, which is defined by

$$F(\mathbf{r}) = \langle \psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle. \tag{2.12}$$

$F(\mathbf{r})$ is the probability amplitude of finding two electrons in the condensed state at point $\mathbf{r}$. It is also called the *Cooper pair amplitude.*

If we assume that the transition temperature T_c of the N-S layer corresponds to a second-order transition, as is indeed observed in most cases, then for $T = T_c$ the $F(\mathbf{r})$ are small everywhere and are ruled by the linear self-consistency equation.

The method of determination of the pair potential $\Delta(x)$ for a layered structure is to guess a shape of $\Delta(x)$, solve the eigenfunction of (2.10) for this potential, insert the solution u,v in the self-consistency requirement (2.11), and obtain the new value for $\Delta(x)$, and iterate the process. In order to have a simpler situation, we shall restrict our attention to the vicinity of the transition point of the layered system and assume that the superconducting transition is always of second order. When this is true, the pair potential Δ is small at all points in space when the temperature is close to the transition point. Then (2.10) can be treated as a perturbation in the eigenvalue equation, and the self- consistency condition (2.11) becomes a linear integral equation for Δ

This equation can be written as

$$\Delta(\mathbf{r}) = \int d^3\mathbf{r}'\Delta(\mathbf{r}')K(\mathbf{r},\mathbf{r}'). \tag{2.13}$$

The kernel is

$$K(\mathbf{r},\mathbf{r}') = N(0)V(\mathbf{r})[\ln(1.14\theta_D/T_c)\delta^3(\mathbf{r}-\mathbf{r}') - X(\mathbf{r}-\mathbf{r}')],$$

with

$$X(\mathbf{r}) = (2\pi)^{-3}\int d^3k e^{i\mathbf{k}\cdot\mathbf{r}}\chi^{-1}(\xi^2k^2),$$

where θ_D is Debye temperature. We then transform the linear integral equation into a differential form

$$\chi(-\xi_T^2\nabla^2)\Delta(\mathbf{r}) = \ln[\frac{T_c(\mathbf{r})}{T_c}]\Delta(\mathbf{r}), \tag{2.14}$$

where $\xi_T = \frac{\hbar D}{2\pi k_B T}$ is a temperature dependent coherence length and $D = \frac{1}{3}v_F l$ is the diffusion coefficient. The function χ can be expressed in term of the digamma function as $\chi(Z) = \psi(\frac{1}{2} + \frac{1}{2}Z) - \psi(\frac{1}{2})$. Equation (2.14) is a Schrödinger like equation, and therefore we are able to make a direct mathematical model which corresponds to the quantum motion of a particle of energy E in a potential $U(\mathbf{r})$.

A simple case is a N-S sandwich layered structure with appropriate boundary conditions in the Cooper limit, $D_N, D_S \ll \xi$. One can find for this situation

$$\frac{T_c}{T_{cs}} \cong [1 + (\frac{\pi^2}{4})(\frac{D_N}{D_S})]^{-1}, \tag{2.15}$$

where $T_{cs} \equiv T_c(\mathbf{r})$ is the bulk transition temperature defined by

$$[N(0)V(\mathbf{r})]^{-1} = \ln(\frac{1.14\theta_D}{T_{cs}}). \tag{2.16}$$

Note the comparison with Cooper's formula

$$\frac{T_c}{T_{cs}} = (\frac{1.14\theta_D}{T_{cs}})^{-D_N/D_S}. \tag{2.17}$$

Due to the fact that the theory agrees with many experimental results, this method is extensively used to investigate properties of the proximity effect.

2.3 McMillan Tunneling Model

The idea of this model is to imagine that there is a potential barrier separating the superconductor and normal metal (S-N sandwich structure) and treat tunneling through this barrier by the tunneling method. The assumptions of this model are: (1). the film of superconductor S of thickness a_S is separated by a potential barrier from the film of normal metal N of thickness a_N. (2). The tunneling Hamiltonian describes the penetration of electrons through the barrier. This restricts the transmission probability of the barrier to be much less that one. (3). The tunneling matrix elements $T_{nn'}$ are equal in magnitude between every state ϕ_n in S and every state $\phi_{n'}$ in N, and there are no momentum conservation selection rules to restrict the magnitudes of $T_{nn'}$. The equal magnitude of $T_{nn'}$ also implies that the relaxation time τ_N for tunneling from N to S is the same for each state ϕ_n' in N. (4). Both N and S layers are thin compared with the characteristic superconducting length so that the properties of each film are uniform across their thickness. This characteristic length is energy dependent, being $\hbar v_F/2E$ at energy E in N, and must be much less than the usual coherence length $\sim \hbar v_F/2\Delta$. (5). The ratio of the mean free path to the film thickness remains constant and ≈ 1 [16] .

The Hamiltonian for the sandwich is the sum of the Hamiltonians for the N and S slabs and the tunneling Hamiltonian, which can be written as

$$H = H_N + H_S + H_T, \tag{2.18}$$

where

$$H_T = \sum_{nn'} T_{nn'}(C^\dagger_{\uparrow n} C_{\uparrow n'} + C^\dagger_{\downarrow -n'} C_{\downarrow -n}) + H.c. \tag{2.19}$$

The electron-phonon interaction and the tunneling Hamiltonian is treated in second-order, self-consistent perturbation theory. The principal results of this model are as follows.

(1). There exists an energy gap in the excitation spectrum $\Delta \sim \hbar/\tau_N$. τ_N is the average time that an electron spends in the normal metal before penetrating the barrier and escaping to the superconductor layer, and $\tau_N = L_N/v_F\sigma$. Here, L_N denotes the average electron path length between collisions with the barrier, σ is the barrier penetration probability, and v_F is the Fermi velocity.

(2). The electronic density of states qualitatively agrees with experimental results. One finds

$$N_{S,N}(E) = Re\{\frac{E}{[E^2 - V_{S,N}^2(E)]^{1/2}}\}, \tag{2.20}$$

where $V_{S,N}(E)$ are the self-energies.

(3). The study of the self-consistency of the BCS potential with a finite pairing interaction in the normal layer shows an enhanced contribution to the measured energy gap, which provides an experimental probe of the paring interaction.

(4). Due to the theory being linear at the transition temperature, we can express the transition temperature T_c in terms of the thickness and the bulk density of states. The transition temperature can be determined by

$$\ln(\frac{T_{cs}}{T_c}) = (\frac{\Gamma_N}{\Gamma})[\psi(-\frac{1}{2} + \Gamma/2\pi T_c) - \psi(-\frac{1}{2})], \tag{2.21}$$

where ψ is the digamma function and T_{cs} denotes the transition temperature of the bulk superconductor, which satisfies

$$1 = \lambda_S \int_0^{\omega_c} \tanh(\frac{E}{2T_{cs}})\frac{dE}{E}.$$

Two limits are of interest. One is the situation for large Γ, which by using $\psi(x) \sim \ln(x)$ for large x results in

$$\frac{T_c}{T_{cs}} \sim (T_{cs}\pi/2\gamma\Gamma)^{\Gamma_S/\Gamma_N}, \tag{2.22}$$

where $\Gamma = \Gamma_S + \Gamma_N$, $\Gamma_S/\Gamma_N = a_N N_N(0)/a_S N_S(0)$, a_N and a_S are the thicknesses of the normal and superconductor layer, $N_N(0)$ and $N_S(0)$ are the bulk density of states of the normal metal and the superconductor, and $\gamma = 1.781$. Another limit of interest is the Cooper limit of thin films, which gives

$$\frac{T_c}{T_{cs}} \sim (T_{cs}\pi/2\gamma\omega_c)^{\Gamma_S/\Gamma_N}, \tag{2.23}$$

where ω_c is the cutoff frequency.

Chapter 5

Single Layer

In this chapter, we introduce a different approach with regard to self-consistency of the pair amplitude. We start with the simplest system, which is a superconducting thin film surrounded by a normal metal. The approach gives the solution of the temperature and thickness dependence of the gap parameter, which is obtained by solving the gap equation from the self-consistency condition imposed on the pair amplitude. The approach provides a general method for the self-consistent solution of the Bogoliubov equations in this particular geometry and will be applied to the infinite superlattice and to the finite superlattice systems.

1 The Energy Eigenstates

The system consists of a clean superconducting film with thickness 2a surrounded by a clean normal metal. The coordinates we choose for such a system are such that the superconductor occupies the region $\mid x \mid< a$ and the normal region at $\mid x \mid> a$. Figure 5.1 shows the system. The Hamiltonian for

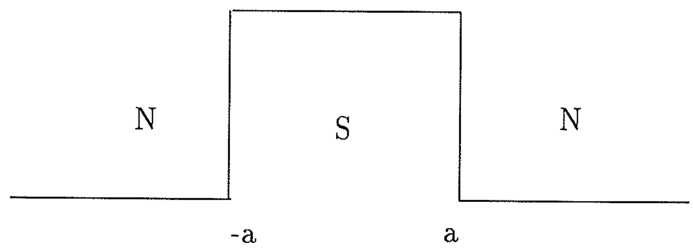

Figure 5.1: Single superconductor layer

such a system can be written as

$$H = \Theta[1 - (\frac{x}{a})]H_1 + \Theta[(\frac{x}{a}) - 1]H_2. \tag{1.1}$$

The operator H_1 refers to the superconductor and the operator in the normal metal is represented by H_2, with H_i, $i = 1, 2$, defined by

$$H_i = \int d^3r\psi^\dagger(\mathbf{r})\epsilon_i(-i\nabla)\psi(\mathbf{r}) - V_i\int d^3r\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}), \tag{1.2}$$

where $\psi_\sigma(\mathbf{r})$ is the second quantized electron field operator and

$$\epsilon_i(-i\nabla) = -\frac{\nabla^2}{2m_i} - \mu_i$$

The coefficients V_i are the phonon induced BCS interaction, and are given by

$$V_1 = V$$

and

$$V_2 = 0.$$

In the mean field approximation, Equation (1.2) can be expressed as

$$\begin{aligned} H_i &= V_i\int d^3r \mid F(x) \mid^2 + \int d^3r\psi^\dagger(\mathbf{r})\epsilon_i(-i\nabla)\psi(\mathbf{r}) \\ &- V_i\int d^3rF(x)[\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})]. \end{aligned} \tag{1.3}$$

The term $F(x)$ is the real spatially dependent pair amplitude $F(\mathbf{r})$, and is given by

$$F(\mathbf{r}) = F(x) = -\langle\psi_\uparrow(x)\psi_\downarrow(x)\rangle. \tag{1.4}$$

$F(x)$ can be obtained by using the quasiparticle creation operators $a^\dagger$ and $b^\dagger$ which operate on the ground state $\mid 0\rangle$. In terms of the Nambu doublet

$$\phi(\mathbf{r}) = \left\{ \begin{array}{c} \psi_\uparrow(\mathbf{r}) \\ \psi_\downarrow^\dagger(\mathbf{r}) \end{array} \right\}, \tag{1.5}$$

from Equation (1.3) we obtain the field equations: for $\mid x \mid < a$, the equation is

$$[i\frac{\partial}{\partial t} - \epsilon_1(-i\nabla)\tau_3 + VF(x)\tau_1]\phi(\mathbf{r},t) = 0, \tag{1.6}$$

and for $\mid x \mid > a$;

$$[i\frac{\partial}{\partial t} - \epsilon_2(-i\nabla)\tau_3]\phi(\mathbf{r},t) = 0, \tag{1.7}$$

where τ_i are the Pauli matrices and $\phi(\mathbf{r},t) = e^{-iHt}\phi(\mathbf{r})e^{iHt}$. The system can now be quantized by imposing the equal time anticommutator

$$\{\phi(\mathbf{r},t), \phi^\dagger(\mathbf{r}',t)\} = \delta(\mathbf{r}-\mathbf{r}'). \tag{1.8}$$

Due to the condition of continuity of the current across the interfaces of the superconductor and normal metal, the boundary condition for Equations (1.6) and (1.7) in general are given by

$$r\phi(\mathbf{r},t) \mid_{|x|=a-\delta} = \phi(\mathbf{r},t) \mid_{|x|=a+\delta},$$

$$t\nabla\phi(\mathbf{r},t) \mid_{|x|=a-\delta} = \nabla\phi(\mathbf{r},t) \mid_{|x|=a+\delta}, \tag{1.9}$$

where $rt = m_2/m_1$ and$\delta \to 0^+$. For convenience we set the transmission and reflection coefficients $t = r = 1$ and assume $m_1 = m_2$. Under the given condition (1.9), we can solve Equations (1.6) and (1.7) by writing the field operator $\phi(\mathbf{r},t)$ as a sum of positive and negative frequency terms:

$$\begin{aligned}\phi(\mathbf{r},t) &= \frac{1}{(2\pi)^3}\sum_{i=1}^{4}\int dE\int d^2l[u^{(i)}(E,l,x)a^{(i)}(E,l)e^{-i(Et-l\cdot\rho)} \\ &+ v^{(i)}(E,l,x)b^{(i)\dagger}(E,l)e^{i(Et-l\cdot\rho)}],\end{aligned} \tag{1.10}$$

where $E > 0$, $\mathbf{l} = (k_y, k_z)$, and $\rho = (y,z)$. The index $i = 1,...,4$ represents the four linearly independent solutions which will be obtained from Equations (1.7) and (1.8). The wave functions $u^{(i)}$ and $v^{(i)}$ satisfy

$$\{E - [-\frac{1}{2m_1}\frac{d^2}{dx^2} + \frac{l^2}{2m_1} - \mu_1]\tau_3 + VF(x)\tau_1\}u^{(i)}(E,l,x) = 0$$

and

$$\{-E - [-\frac{1}{2m_1}\frac{d^2}{dx^2} + \frac{l^2}{2m_1} - \mu_1]\tau_3 + VF(x)\tau_1\}v^{(i)}(E,l,x) = 0 \tag{1.11}$$

for $\mid x \mid < a$, where $l^2 = \mathbf{l}\cdot\mathbf{l} = k_y^2 + k_z^2$, and

$$\{E - [-\frac{1}{2m_2}\frac{d^2}{dx^2} + \frac{l^2}{2m_2} - \mu_2]\tau_3\}u^{(i)}(E,l,x) = 0$$

and

$$\{-E - [-\frac{1}{2m_2}\frac{d^2}{dx^2} + \frac{l^2}{2m_2} - \mu_2]\tau_3\}v^{(i)}(E,l,x) = 0 \tag{1.12}$$

for $\mid x \mid > 0$.

The normalization condition are

$$\int_{-\infty}^{\infty} dx\overline{u}^{(i)}(E,l,x)u^{(j)}(E,l,x) = 2\pi\delta_{ij}\delta(E-E'),$$

$$\int_{-\infty}^{\infty} dx\overline{v}^{(i)}(E,l,x)u^{(j)}(E,l,x) = 2\pi\delta_{ij}\delta(E-E'),$$

and

$$\int_{-\infty}^{\infty} dx\overline{u}(E,l,x)v^{(j)}(E,l,x) = 0. \tag{1.13}$$

The anticommutation relation implies

$$\{a^{(i)}(E,l), a^{(j)}(E,l)^\dagger\} = (2\pi)^3\delta_{ij}\delta(E-E')\delta(\mathbf{l}-\mathbf{l}')$$

and

$$\{b^{(i)}(E,l), b^{(j)}(E,l)^\dagger\} = (2\pi)^3\delta_{ij}\delta(E-E')\delta(\mathbf{l}-\mathbf{l}'), \tag{1.14}$$

with all other anticommutators vanishing. Now, the boundary conditions for the wave functions are

$$u^{(i)}(E,l,x)\mid_{|x|=a-\delta} = u^{(i)}(E,l,x)\mid_{|x|=a+\delta},$$

$$v^{(i)}(E,l,x)\mid_{|x|=a-\delta} = v^{(i)}(E,l,x)\mid_{|x|=a+\delta},$$

$$\frac{du^{(i)}(E,l,x)}{dx}\mid_{|x|=a-\delta} = \frac{du^{(i)}(E,l,x)}{dx}\mid_{|x|=a+\delta},$$

and

$$\frac{dv^{(i)}(E,l,x)}{dx}\mid_{|x|=a-\delta} = \frac{dv^{(i)}(E,l,x)}{dx}\mid_{|x|=a+\delta}.$$

Therefore, given a solution $u^{(i)}(E,l,x)$ to Equations (1.10) and (1.11) satisfying the appropriate normalization and boundary conditions, we can write the corresponding solution $v^{(i)}(E,l,x)$, which also satisfies the normalization and boundary conditions by using

$$v^{(i)}(E,l,x) = u^{(i)}(-E,l,x).$$

In order to find the solution of Equation (1.10), we introduce the approximation for the pair amplitude which in the domain of the thin film is homogeneous:

$$VF(x) = \Delta(x) \tag{1.15}$$

for $\mid x \mid < a$. Under this assumption, Equation (1.12) can be solved exactly and the pair amplitude $F(x)$ can be evaluated as a function of the order parameter

$\Delta(x)$. The order parameter is determined self-consistently by requiring

$$\Delta(x) = \frac{V}{2a}\int_{-a}^{a} F(x,\Delta)dx. \tag{1.16}$$

Assuming that both superconducting and normal metal have the same parameters m and k_F, and also that the transmission and reflection coefficient are unity, we can write the Bogoliubov Equation (1.10) as

$$\{E + \frac{\tau_3}{2m}[\frac{d^2}{dx^2} + q^2] + \Delta(x)\tau_1\}u(E,l,x) = 0, \tag{1.17}$$

with

$$\Delta(x) = \begin{cases} \Delta & -a < x < a \\ 0 & x < -a \text{ or } x > a \end{cases}$$

and $q^2 = k_F^2 - (k_y^2 + k_z^2)$. Let us define

$$u(E,l,x) = \varphi(E,l,x)e^{iqx},$$

by which the equation becomes

$$\{E + \frac{\tau_3}{2m}[\frac{d^2}{dx^2} + 2iq\frac{d}{dx}] + \Delta(x)\tau_1\}\varphi(E,l,x) = 0. \tag{1.18}$$

If $\varphi(E,l,x)$ is smooth on the atomic scale, we can drop the second derivative term in the above equation, and obtain

$$\{E + i\frac{\tau_3 q}{m} + \Delta(x)\tau_1\}\varphi(E,l,x) = 0. \tag{1.19}$$

The general solution of the equation can be written as

$$\varphi_\pm(E,l,x) = \begin{cases} B_\pm \begin{bmatrix} 1 \\ 0 \end{bmatrix} e^{ikx} \pm B_\pm^* \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-ikx} & \text{for } \mid x \mid > a, \\ A_\pm \begin{bmatrix} 1+\gamma \\ \delta \end{bmatrix} e^{ipx} \pm A_\pm^* \begin{bmatrix} \delta \\ 1+\gamma \end{bmatrix} e^{-ipx} & \text{for } \mid x \mid < a, \end{cases} \tag{1.20}$$

where $\gamma = (1-\delta^2)^{1/2}$ and $\delta = -\Delta/E$. Detailed information on solving this equation can be found in Ref.[22]. Being able to find the pair amplitude $F(x)$, we now turn to evaluate the self-consistent gap equation.

2 The Pair Amplitude and the Self-Consistent Gap Equation

In this section we use the eigenfunctions just derived to evaluate the pair amplitude $F(x)$ and determine the self- consistent gap Equation (1.16). The pair amplitude may be obtained from

$$F(x) = -\langle\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle = -\langle\phi(\mathbf{r})\phi^\dagger(\mathbf{r})\rangle_{12},$$

where the subscript "12" refers to the 1-2 component of the matrix formed from outer product of $\phi(\mathbf{r})$ with $\phi^\dagger(\mathbf{r})$. The angular bracket denote a thermal average.

The pair amplitude can be written

$$F(x) = -\sum_{i=1}^{4}\int_0^{\omega_d}\frac{dE}{2\pi}\int\frac{d^2l}{(2\pi)^2}[u^{(i)}(E,l,x)\overline{u}^{(i)}(E,l,x)]_{12}\times\tanh(\frac{\beta E}{2}). \quad (2.21)$$

In principle, it is possible to consider the general case and calculate the pair amplitude from (2.21) by using the eigenfunction u. Except in certain limiting cases, the resultant solutions are fairly complicated so that only a numerical analysis is possible. One limiting case of $m_1 = m_2 = m$, $r = t = 1$ and $\mu_1 = \mu_2 = \mu$ provides a relatively simple solution. It is hoped that small departures from these limits would introduce small quantitative corrections to the results, so that a relatively good qualitative analysis should be obtained.

Some manipulation of (2.21) gives for the pair amplitude $F(x)$, for$|x| < a$,

$$F(x) = \frac{m\Delta}{2\pi^2}\int_0^{k_F} dq \int_0^{\omega_d} \frac{dE}{E}[1 - \frac{\cos(2pa)\cos(2px)}{1-\delta^2\cos^2(2pa)}]\tanh(\frac{\beta E}{2}), \qquad (2.22)$$

and from the self-consistency gap requirement (1.16), the gap equation for the case $x < -a$,

$$\frac{1}{VN(0)} = \int_0^{\omega_d}\frac{dE}{E}\int_0^{k_F}\frac{dq}{k_F}[\frac{1}{1-\delta^2\cos^2(2pa)}](1 - \frac{\sin 4pa}{4pa})\tanh(\frac{\beta E}{2}), \quad (2.23)$$

where $N(0) = mk_F/2\pi^2$ is the density of states at the Fermi surface of the normal metal for one spin projection.

3 Thickness Dependence of the Transition Temperature

We now calculate the dependence of the transition temperature $T_c(a)$ on the thickness of the film. In the limit $\Delta \to 0$, Eq.(2.22) simplifies considerably and it is possible to obtain analytical results as $T \to 0$ as well as the asymptotic form of $T_c(a)$ as $a \to \infty$. Considering the limit $\Delta \to 0$, the gap equation becomes

$$1 = VN(0)\int_0^{\omega_d}\frac{dE}{E}\tanh(\frac{\beta E}{2})\int_0^{k_F} dq[1 - \frac{\sin(4ka)}{4ka}], \qquad (3.24)$$

where $k = mE/q$. Equation (3.24) determines the transition temperature $T_c(a)$ for a given thickness of film, a. First let us define

$$I(\omega) = \frac{1}{k_F}\int_0^{\omega}\frac{dE'}{E'}\int_0^{k_F} dq[1 - \frac{\sin(4ka)}{4ka}]. \qquad (3.25)$$

Assuming that $T_c(a) \ll \omega_d$, and integrating (2.26) by parts, we get

$$1 = VN(0)\{I(\omega_d) - \frac{\beta}{2}\int_0^{\infty} d\omega I(\omega)\cosh^{-2}(\frac{\beta\omega}{2})\}. \qquad (3.26)$$

The first term in Equation (3.26) represents the zero temperature contribution to the gap function, and the second term contains the thermal corrections. The function $I(\omega)$ may be calculated to give

$$I(\omega) = I(\Lambda\Omega),$$

where

$$\Lambda = 2k_F a,$$

$$\Omega = \omega/E_F, \tag{3.27}$$

and $I(x)$ is given by

$$I(x) = \gamma_e + \ln x + \frac{1}{2}[\frac{\sin x}{x} - \cos x - 2Ci(x) - xSi(x)]. \tag{3.28}$$

$Ci(x)$ and $Si(x)$ are the Cosine and Sine integrals, details of which are given in Appendix A, and γ_e is Euler's constant. In the limit $x \to \infty$ and $x \to 0$, we can obtain the following approximations:

$$\lim_{x\to\infty} I(x) = \gamma_e + \ln x + O(1/x), \tag{3.29}$$

and

$$\lim_{x\to 0} = \frac{\pi x}{4} + O(x^2). \tag{3.30}$$

We next define the critical thickness a_c as the thickness below which it is not possible to maintain the superconducting state at any temperature,

$$T_c(a_c) = 0.$$

This can be determined from the gap function by setting $T = 0$, for which $I(x) = I(\Lambda_c\Omega_d)$, with ω_d the Debye frequency. Assuming that $\Lambda_c\Omega_d \gg 1$, and using (3.29), in the limit $T = 0$ we obtain

$$a_c = \frac{1}{\pi k_F}(\frac{T_F}{T_c}), \tag{3.31}$$

where $T_F = E_F/k_B$ denotes the Fermi temperature and T_c is the bulk superconductor transition temperature. This result can be written in terms of the coherence length

$$a_c = \frac{\pi e^{-\gamma_e}}{2}\xi_0 \approx 0.882\xi_0, \tag{3.32}$$

where $\xi_0 = v_F/\pi\Delta_0$ and Δ_0 is the bulk zero temperature gap.

In the finite temperature case, using (3.38) for a_c, one can obtain the function for $T_c(a)$ from (3.32)

$$\ln(\frac{\Lambda}{\Lambda_c}) = \frac{1}{2\tau_c}\int_0^\infty ds I(s)\cosh^{-2}\frac{s}{2\tau_c}, \tag{3.33}$$

where

$$\tau_c = \Lambda\frac{T_c(a)}{T_F} = \frac{\Lambda}{\Lambda_c}\frac{T_c(a)}{T_c}\frac{2}{\pi}.$$

There are two limiting cases of interest.

(1). In the limit $\tau_c \ll 1$, by using (3.30), we obtain

$$\lim_{a\to a_c}\frac{T_c(a)}{T_c} \sim \frac{1}{\ln 2}\frac{a_c}{a}\ln(\frac{a}{a_c}). \tag{3.34}$$

Expanding the above equation around $a/a_c = 1$, we find

$$\lim_{a\to a_c}\frac{T_c(a)}{T_c} \sim (\frac{a}{a_c} - 1)\frac{1}{\ln 2} \approx 1.443(\frac{a}{a_c} - 1). \tag{3.35}$$

(2). In the limit $\tau_c \gg 1$, we have

$$\lim_{a\to\infty}\frac{a}{a_c} \sim \frac{\pi^2}{16}\frac{T_c}{T_c(a)}\frac{1}{\ln(T_c/T_c(a))}. \tag{3.36}$$

Expending around $T_c/T_c(a) = 1$ to first order results in

$$\lim_{a\to\infty}\frac{T_c(a)}{T_c} \sim 1 - \frac{\pi^2}{16}\frac{1}{a/a_c} \approx 1 - \frac{0.617}{(a/a_c)}. \tag{3.37}$$

Such results can be compared with Zaitsev's results obtained using the Ginzburg-Landau theory [22]. Figure 5.2 shows the dependence of the critical temperature on film thickness.

Now we write the equation governing the transition temperature in a more general form. The gap function of Eq. (3.24) can be rewritten as

$$\begin{aligned} 1 &= VN(0)\int_0^{\omega_d}\frac{dE}{E}\int_0^{k_F}dq[1-\frac{\sin(4ka)}{4ka}] \\ &+ VN(0)\int_0^{\omega_d}\frac{dE}{E}[\tanh(\frac{\beta E}{2})-1]\int_0^{\omega_d}dq[1-\frac{\sin(4ka)}{4ka}]. \end{aligned} \quad (3.38)$$

Assuming $T_d \gg T_c(a)$, we extend the limit on the E integral in the second term of this equation to ∞, and find the resulting equivalent equations:

$$\ln(\frac{a}{a_c}) = \frac{\pi}{2}\tau_c \ln 2 - \frac{1}{2}\int_0^1 dt(1-\frac{1}{t})^2[1-\frac{\pi\tau_c t}{\sinh(\pi\tau_c t)}] \quad (3.39)$$

or

$$\ln[\frac{T_c}{T_c(a)}] = \frac{\pi}{8\tau_c} + \frac{1}{2}\int_1^\infty dt(1-\frac{1}{t^2})\ln\tanh(\frac{\pi\tau_c t}{2}). \quad (3.40)$$

The equations generated in this manner lead to the same asymptotic limits, (3.34) and (3.36), as was used earlier to derive them. The numerical equivalence of handing the cutoff dependence in this manner will be useful to evaluate the gap equation with a finite order parameter Δ.

One interesting property is the thickness dependence of the gap, $\Delta(a)$. Setting $T = 0$, the gap function (2.24) gives

$$\frac{1}{VN(0)} = \frac{1}{k_F}\int_0^{\omega_d} dE\int_0^{k_F} dq\frac{E}{E^2-\Delta^2\cos^2(2pa)}[1-\frac{\sin(4pa)}{4pa}]\tanh(\frac{\beta E}{2}), \quad (3.41)$$

which can be written as

$$\ln(\frac{a}{a_c}) = \kappa_0[G_1(\kappa_0)+G_2(\kappa_0)], \quad (3.42)$$

where

$$\kappa_0 = \frac{\Lambda}{\Lambda_c}\frac{\Delta_0(a)}{\Delta_0}e^{-\gamma_e}$$

and the functions $G_1(\kappa_0)$, $G_2(\kappa_0)$ are defined as

$$G_1(\kappa_0) = \int_0^\infty dy \int_{\kappa_0 y}^\infty \frac{dx}{x^2} \frac{\sin^2 x}{y^2 + \sin^2 x}[1 - \frac{\sin 2x}{2x}], \quad (3.43a)$$

$$G_2(\kappa_0) = \int_0^1 dy \int_{\kappa_0 y}^\infty \frac{dx}{x^2} \frac{y^2}{y^2 + \sinh^2 x}[1 - \frac{\sinh 2x}{2x}]. \quad (3.43b)$$

The upper limit of the integration is set to ∞ due to the large ratio $E_d/\Delta_0(a)$. Numerical solution of (3.42) provides the behavior of the thickness dependence of the zero temperature gap; for details, see Ref.[22].

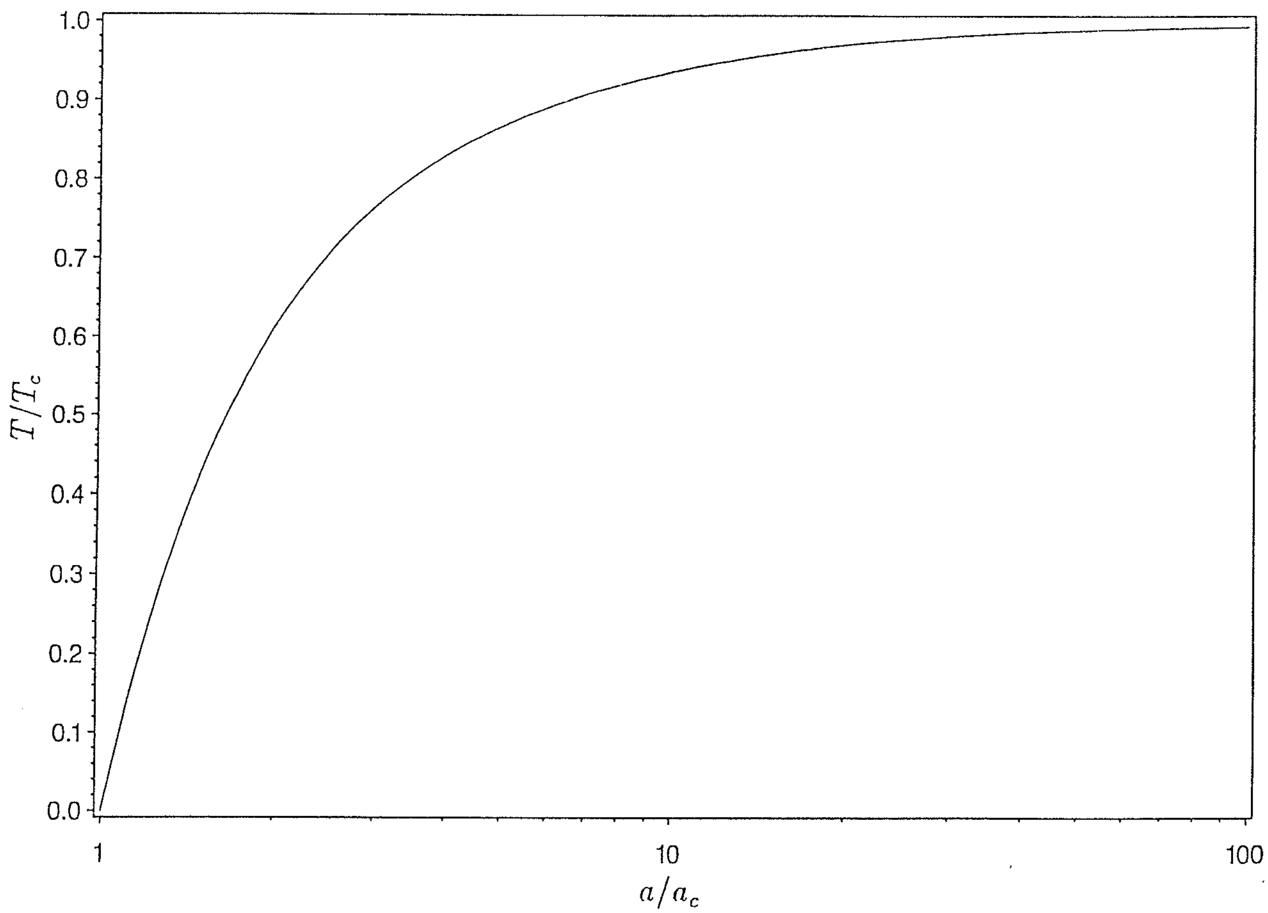

Figure 5.2: The dependence of the reduced temperature $T(a)/T_c$ on the thickness for single film

Chapter 6

The Superlattice

In this chapter, following the line of approach introduced in the last chapter, we present the calculation of the critical temperature for an infinite superlattice system with incorporates explicitly its inherent Bloch nature. A comparison can be made with other bilayer approximations, which indicates the most notable differences among the approaches arise in the Cooper limit of thin films.

1 Definition of the Superconducting Superlattice

The system we study consists of clean alternating layer in the x direction of two different superconductors. We assume that the Fermi velocity, effective masses and Debye temperatures are identical in both layers. The thickness of superconductor 1 is denoted by a_1 and that of 2 by a_2. Figure 6.1 shows the basic superlattice system. The general method we apply to the system is based on the Bogoliubov equations using a step function approximation for the pair amplitude, the height of the amplitude then being determined by a minimization of the free energy of the system. This technique is analogous to that used in the single film geometry.

S_1	S_2	S_1	S_2	S_1	S_2	...

Figure 6.1: The Superlattice System

The Hamiltonian for the system can be written as

$$\begin{aligned} H &= \int d^3r g(x) \mid F(x) \mid^2 \\ &\quad + \int d^3r \phi^\dagger(r)[-(1/2m)\nabla^2 - \mu]\tau_3\phi(r) \\ &\quad - \int d^3r g(x) F(x) \phi^\dagger(r)\tau_1\phi(r), \end{aligned} \tag{1.1}$$

where

$$\phi(r) = \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{pmatrix},$$

$$F(x) = F^*(x) = -\langle\psi_\uparrow(r)\psi\downarrow(r),\rangle$$

and $g(x)$ is the spatially inhomogeneous BCS coupling constant. The pair potential defined as $\Delta(x) = g(x)F(x)$ results from the equation of motion for the wave function $u(E,x)$:

$$[E + i(q/m)\tau_3\frac{d}{dx} + \Delta(x)\tau_1]u(E,x) = 0, \tag{1.2}$$

$q = \sqrt{k_F^2 - k_y^2 - k_z^2}$, k_y and k_z being the momentum in the y and z direction. We assume that $g(x)$ is the bulk value g_1 or g_2 in the respective regions. The step function approximations for the pair potential are

$$\Delta(x) = \begin{cases} \Delta_1 & \text{in } S_1 \\ \Delta_2 & \text{in } S_2 \end{cases} \tag{1.3}$$

The parameters Δ_1, Δ_2 are determined by a minimization of the free energy of the system:

$$\langle\frac{\partial H}{\partial \Delta_1^2}\rangle = \langle\frac{\partial H}{\partial \Delta_2^2}\rangle = 0,$$

which can be written as follows:

$$\begin{aligned}\Delta_1 &= \frac{1}{a_1}\int_{-a_1}^{0} dx g_1 F(x),\\ \Delta_2 &= \frac{1}{a_2}\int_{0}^{a_2} dx g_2 F(x).\end{aligned} \tag{1.4}$$

The general solution of Eq (1.2) can be written as:

$$u(E,x) = \begin{cases} A_1\begin{pmatrix}1+\gamma_1\\ \delta_1\end{pmatrix} e^{ip_1x} + B_1\begin{pmatrix}\delta_1\\ 1+\gamma_1\end{pmatrix} e^{-ip_1x} & \text{in } S_1\\ A_2\begin{pmatrix}1+\gamma_2\\ \delta_2\end{pmatrix} e^{ip_2x} + B_2\begin{pmatrix}\delta_2\\ 1+\gamma_2\end{pmatrix} e^{-ip_2x} & \text{in } S_2\end{cases} \tag{1.5}$$

The parameters are defined as: $\delta_i = -\frac{\Delta_i}{E}$, $\gamma_i = \sqrt{1-\delta_i^2}$, $p_i = \gamma_i mE/q$, $i = 1,2$. The coefficients A_i, B_i are determined by the normalization condition

$$\int_{-\infty}^{\infty} dx u^*(E',x)u(E,x) = 2\pi\delta(E-E'), \tag{1.6}$$

by continuity at the interface, and by the requirement of Bloch's theorem $u(x) = e^{iqd}u(x+d)$ for periodic systems, where $d = a_1 + a_2$ is the lattice period and q is the Bloch wavevector. For a nontrivial solution we have

$$\cos(dq) = \cos(a_1p_1)\cos(a_2p_2) - [1-(1-\delta_1\delta_2)/\gamma_1\gamma_2]\cdot\sin(a_1p_1)\sin(a_2p_2). \tag{1.7}$$

These conditions serve to determine the unknown coefficients. Having done so, we are able to evaluate the self- consistency equation.

2 Calculation of $T_c(a_1, a_2)$

Generally the self-consistency equations will be difficult to solve. In order to calculate the thickness dependent transition temperature $T_c(a_1, a_2)$, we take the limits that Δ_1 and Δ_2 approach zero, in which case (1.7) becomes $\cos(dq) = \cos(dmE/q)$. In such a limit the gap equations also simplify and the transition temperature is determined from

$$\begin{aligned}
\ln(\frac{a_1}{a_{c1}})\ln(\frac{a_2}{a_{c2}}) &= \ln(\frac{a_1}{a_{c1}})[I(r\rho) - J(r\rho, 1/r)] \\
&+ \ln(\frac{a_2}{a_{c2}})[I(\rho) - J(\rho, r)] \\
&- [I(\rho) - J(\rho, r)][I(r\rho) - J(r\rho, 1/r)] \\
&+ [J(\rho, r) - K(\rho)][j(r\rho, 1/r) - K(r\rho)], \qquad (2.8)
\end{aligned}$$

where the parameters are defined as follows:

$$\rho = \frac{2}{\pi}\frac{a_1}{a_{c1}}\frac{T_c(a_1, a_2)}{T_{c1}}, \qquad r = \frac{a_1}{a_2}$$

and

$$a_{c1} = \frac{1}{\pi k_F}\frac{T_F}{T_{c1}}, \qquad a_{c2} = \frac{1}{\pi k_F}\frac{T_F}{T_{c2}},$$

where T_{c1} and T_{c2} are the bulk critical temperature for S_1 and S_2 and a_{c1} and a_{c2} are the critical thickness at which the transition temperature vanishes. The functions appearing in (2.8) are defined as

$$\begin{aligned}
I(x) &= \frac{1}{2}\pi x \ln 2 - x\int_0^\infty \frac{dz}{z^2}[\frac{\sin(2z)}{2z}]\ln[1 + \exp(-2z/x)], \\
J(x, y) &= x\int_0^\infty \frac{dz}{z^3}\sin^2 z \cot[z(1+y)]\ln\cosh(z/x), \\
K(x) &= \frac{1}{2}x\int_0^\infty \sin(2z)\ln\cosh(z/x). \qquad (2.9)
\end{aligned}$$

Note that if we consider the case $g_2 = 0$, then (2.8) can be reduced to

$$\ln(\frac{a_1}{a_{c1}}) = \ln(\rho) - J(\rho, r). \qquad (2.10)$$

For infinite a_2, the function $J(\rho, r)$ vanishes, and an analysis of the other term yields the solution $T_c(a_{c1}) = 0$. From this one can see that $J(\rho, r)$ represents coherence effects the other layers introduce to the single film geometry.

From Equations (2.8) and (2.9) the transition temperature can be obtained for the cases of $g_2 \neq 0$ and $g_2 = 0$. The results of the numerical analysis for various values of b/b_c can be found in Ref.[36].

Now we compare the results with other bilayer approximations in the Cooper limit. It is know that in this limit the de Gennes- Werthamer approaches are unable to completely account for the observed behavior of the transition temperature [37, 38, 39]. The difference between the approaches can readily be seen in the situation $g_2 = 0$. Under such a condition Wethamer's result, described in Chapter 4, becomes

$$\frac{T_c(a_1, a_2)}{T_{c1}} \approx [1 + \frac{\pi^2}{4}(\frac{a_1}{a_2})], \tag{2.11}$$

and the result of de Gennes's is

$$\frac{T_c(a_1, a_2)}{T_{c1}} = (\frac{T_{c1}}{1.14\omega_d})^{(a_1/a_2)}. \tag{2.12}$$

As we can see from these expressions, for a fixed ratio a_1/a_2, as the thickness a_1 tends to zero the critical temperature approaches a finite constant. On the other hand, Eq. (2.14) yields the result

$$\frac{T_c(a_1, a_2)}{T_{c1}} \approx (\frac{a_1}{a_{c1}})^{(a_2/a_1)}. \tag{2.13}$$

This expression for fixed a_1/a_2 tends to zero as a_1 vanishes. This behavior is the same as the McMillan model [40].

In the situation of two different superconductors ($g_2 \neq 0$), taking the thin film limit of (2.8) results in

$$\frac{T_c(a_1, a_2)}{T_{c1}} = (\frac{T_{c2}}{T_{c1}})^{a_2/(a_1+a_2)}, \tag{2.14}$$

valid for a_1/a_{c1} and a_2/a_{c2} but not for $\frac{T_{c2}}{T_{c1}}$ small. Again, this is the same result as in the McMillan model, and differs with the de Gennes-Werthamer approaches.

We can define an effective BCS coupling constant for the geometry as

$$(\frac{1}{gN(0)})_{eff} = \frac{a_1}{a_1+a_2}(\frac{1}{gN(0)})_1 + \frac{a_2}{a_1+a_2}(\frac{1}{gN(0)})_2, \tag{2.15}$$

where the subscripts "1"and "2" indicate S_1 and S_2 bulk values: note that this involves factors of $1/gN(0)$ rather than $gN(0)$ as Cooper and de Gennes used (see Chapter 4). Substituting (2.15) into the BCS expression for the critical temperature gives

$$T_c(a_1, a_2) = 1.14\omega_d \exp\{-[1/gN(0)]_{eff}\}, \tag{2.16}$$

which is the same as (2.14). One can readily see that this inverse Cooper argument highlights the similarities and differences between the Cooper, the de Gennes- Werthamer approaches and the approach we employ.

A comparison with the McMillan model also can be made [36], which is favourable. This is surprising in light of the fact that in this method we assume clean materials with ideal interfaces, while the McMillan model assumes dirty materials with tunneling interfaces.

3 Infinite Superconducting Superlattice

As a check on the methods we will later use for a finite superlattice, in this section we consider an infinite superlattice as the limit of a finite system, and compare the results with the last section.

The system we consider contains superconducting layers S_2 alternating with other superconducting layers S_1. The width of each S_2 film is 2a, and that of S_1 is 2b. The center film is S_2. The energy gaps in all S_1 films are the same and denoted by Δ_1, and those in all S_2 films the same as well, and denoted by Δ_2. Figure 6.2 shown the geometry for the system. Let us first consider a finite number of S_2 layers, N, and then take the limit $N \to \infty$, comparing these results with the infinite superlattice of the last section. As before, we assume that all physical properties, such as Fermi velocity, effective mass, etc., are the same in both superconducting layers.

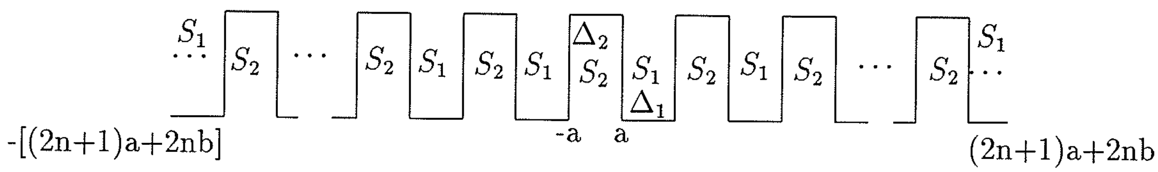

Figure 6.2: Infinite superlattice system

The basic equation for the problem is

$$[E + i(q/m)\tau_3 \frac{d}{dx} + \Delta(x)\tau_1]u(E,x) = 0, \tag{3.17}$$

and the gap equations are

$$\Delta_1 = \frac{1}{a}\int_0^a dx g_1 F(x), \qquad \Delta_2 = \frac{1}{b}\int_0^b dx g_2 F(x). \tag{3.18}$$

Due to the parity symmetry $\varphi(x) \to \tau_1\varphi(-x)$, we can split the solution into two parity states, so that we only need to consider the solution for $x > 0$. Then the solution of Eq.(3.17) for this system will be

$$\begin{aligned}
\varphi_\pm(x) &= A_\pm \begin{pmatrix} 1+\gamma_1 \\ \delta_1 \end{pmatrix} e^{ip_1 x} \pm A_\pm \begin{pmatrix} \delta_1 \\ 1+\gamma_1 \end{pmatrix} e^{-ip_1 x} \\
&= B_\pm \begin{pmatrix} 1+\gamma_2 \\ \delta_2 \end{pmatrix} e^{ip_2(x-d)} \pm C_\pm \begin{pmatrix} \delta_2 \\ 1+\gamma_2 \end{pmatrix} e^{-ip_2(x-d)}
\end{aligned}$$

$$
\begin{aligned}
&= D_{\pm}\begin{pmatrix} 1+\gamma_1 \\ \delta_1 \end{pmatrix} e^{ip_1(x-2d)} \pm E_{\pm}\begin{pmatrix} \delta_1 \\ 1+\gamma_1 \end{pmatrix} e^{-ip_1(x-2d)} \\
&= F_{\pm}\begin{pmatrix} 1+\gamma_2 \\ \delta_2 \end{pmatrix} e^{ip_2(x-3d)} \pm G_{\pm}\begin{pmatrix} \delta_2 \\ 1+\gamma_2 \end{pmatrix} e^{-ip_2(x-3d)} \\
&= \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
&= Y_{\pm}\begin{pmatrix} 1+\gamma_2 \\ \delta_2 \end{pmatrix} e^{ip_2(x-Nd)} \pm Z_{\pm}\begin{pmatrix} \delta_2 \\ 1+\gamma_2 \end{pmatrix} e^{-ip_2(x-Nd)}, \qquad (3.19)
\end{aligned}
$$

with $N = 2n+1$, $d = a+b$ and the parameters δ_i, p_i, γ_i defined as before. The solutions for $x < 0$ are obtain by

$$\varphi_{\pm}(-x) = \pm\tau_1\varphi_{\pm}(x).$$

The coefficients in (3.18) are determined by applying the boundary conditions and the normalization condition. Generally we can find

$$
\begin{aligned}
\mid B_{\pm} \mid^2 &= \mid C_{\pm} \mid^2 \\
\mid D_{\pm} \mid^2 &= \mid E_{\pm} \mid^2 \\
\mid F_{\pm} \mid^2 &= \mid G_{\pm} \mid^2 \\
\vdots &= \vdots \\
\mid Y_{\pm} \mid^2 &= \mid Z_{\pm} \mid^2 . \qquad (3.20)
\end{aligned}
$$

Considering the general situation, we define the following coefficients:

$$
\begin{aligned}
S_{\pm}^{(j)} &= a_{\pm}^{(j)} e^{is_{\pm}^{(j)}} \\
T_{\pm}^{(j)} &= a_{\pm}^{(j)} e^{it_{\pm}^{(j)}} \\
F_{\pm}^{(j)} &= b_{\pm}^{(j)} e^{if_{\pm}^{(j)}} \\
G_{\pm}^{(j)} &= b_{\pm}^{(j)} e^{ig_{\pm}^{(j)}}, \qquad (3.21)
\end{aligned}
$$

with $j = 0, 1, 2, 3, \ldots, n$, $S_\pm^{(j)}$, $T_\pm^{(j)}$ referring to S_1 and $F_\pm^{(j)}$, $G_\pm^{(j)}$ referring to S_2. We find the following condition:

$$S_\pm^{(0)} = T_\pm^{(0)} = A_\pm,$$

and the series terminates when $j = n$. From Eq. (3.20), and applying the boundary conditions to the general expression in terms of $S_\pm^{(j)}$, $T_\pm^{(j)}$, $F_\pm^{(j)}$ and $G_\pm^{(j)}$, one can find the contribution of the center film to the pair amplitude, $\langle \psi_\uparrow(x)\psi_\downarrow(x) \rangle$, as

$$2 \mid A_\pm \mid^2 (1+\gamma_1)[\delta_1 \pm \frac{\sin 2p_1 a}{2p_1 a}]. \tag{3.22}$$

From the normalization requirement

$$\int_{-\infty}^{\infty} \varphi^*(x, E')\varphi(x, E)dx = 2\pi\delta(E - E'),$$

we can find

$$\mid A_\pm \mid^2 = \frac{m}{4 \mid q \mid} \frac{1}{\gamma_2(1+\gamma_2)}. \tag{3.23}$$

Thus, we can express $\mid A_\pm \mid^2$ in terms of the known parameter $\mid Y_\pm \mid^2$. Considering the case $\Delta \to 0$ and finding the amplitudes $\mid a_\pm^{(j)} \mid^2$, $\mid b_\pm^{(j)} \mid^2$ and the phases coefficient $f_\pm^{(j)}$, $s_\pm^{(j)}$ at $\Delta = 0$, then $\mid A_\pm \mid^2$ can be written in term of k, a, b and j. Substituting $\mid A_\pm \mid^2$ to the gap Equations (3.17), we find in the limit $N \to \infty$

$$\begin{aligned} \frac{1}{gN(0)} &= \int_0^{\omega_d} \frac{dE}{E} \int_0^{k_F} dq[1 - \frac{\sin 4ka}{4ka} \tanh(\frac{\beta E}{2})] \\ &+ 2\sum_{j=0}^{\infty} \int_0^{\infty} \frac{dE}{E} \int_0^{k_F} \frac{dq}{k_F} \frac{\sin 2ka}{2ka} \{\sin 2ka \cot 2kd \\ &+ [1 - \frac{\Delta_2}{\Delta_1}] + \frac{\Delta_2}{\Delta_1} \cos 2k4a\} \tanh(\frac{\beta E}{2}). \end{aligned} \tag{3.24}$$

One sees that the first term on the right hand side has been solved already in the single film case, with the result $\gamma + \ln \Lambda\Omega_d$. For the remaining terms, we can shift $E \longrightarrow qE/2ma$ and do the q integration, and use

$$\frac{1}{g_i N(0)} = \gamma + \ln \Lambda_c \Omega_d,$$

where $\Lambda_c = 2a_c k_F = \frac{2}{\pi}\frac{T_F}{T_{ci}}$. The simultaneous gap equations then can be obtained as

$$\begin{aligned}
\ln(\frac{a}{a_c})\ln(\frac{b}{b_c}) &= \ln(\frac{a}{a_c})[I(r\rho_1) - J(r\rho_1, 1/r)] \\
&+ \ln(\frac{b}{b_c})[I(\rho_1) - J(\rho_1, r)] \\
&- [I(\rho_1) - J(\rho_1, r)][I(r\rho_1) - J(r\rho_1, 1/r)] \\
&+ [J(\rho_1, r) - K(\rho_1)][J(r\rho_1, 1/r) - K(r\rho_1)], \qquad (3.25)
\end{aligned}$$

with

$$\rho_1 = \frac{2}{\pi}\frac{a}{a_c}\frac{T_c(a,b)}{T_{c1}}, \qquad r = \frac{b}{a}.$$

The functions are defined as follows:

$$\begin{aligned}
I(x) &= \frac{1}{2}\pi x \ln 2 - x\int_0^\infty \frac{dz}{z^2}[\frac{\sin(2z)}{2z}]\ln[1 + \exp(-2z/x)], \\
J(x, y) &= x\int_0^\infty \frac{dz}{z^3}\sin^2 z \cot[z(1+y)]\ln\cosh(z/x), \\
K(x) &= \frac{1}{2}x\int_0^\infty \sin(2z)\ln\cosh(z/x). \qquad (3.26)
\end{aligned}$$

We immediately see that Equation (3.25) is the same as Equation (2.8), with the exchange of the indices a_2 to b and ρ to ρ_1. This indicates that in the context of this method an infinite superconducting superlattice system can be treated as the limit of a finite number of layers.

Chapter 7

Finite Superlattice System

The last application of the method is to a finite superlattice system which is composed of alternating normal and superconducting layers. We consider a clean superlattice with $l \gg \xi(T)$, where l is the mean free path and $\xi(T)$ is the temperature dependent coherence length. The method we use is the same as before which is based on the Bogoliubov equations using a step function approximation for the pair amplitude, the height of the amplitude determined by a minimization of the free energy of the system:

$$\langle \frac{\partial H}{\partial [\Delta^{(j)}]^2} \rangle = 0,$$

where $\Delta^{(j)}$ is the gap parameter of the j^{th} superconducting region.

The system is composed of layers of identical superconductors of width $2a$ separated by layers of normal metal of width $2b$, while the end of the system is a normal layer. Figure 7.1 shows the system. The S and N represent the superconductor layers and the normal metal layers. The origin of the system is at the center so that the system is symmetric about the origin, and because of parity, we only need to solve one side of the system ($x > 0$), The coordinates we choose for each superconducting layers are from $(2n-1)a+2nb$

to $(2n+1)a+2nb$, with $n = 0, 1, 2, 3 \ldots, n-1$. If N represents the number of superconducting layers, then $N = (2n+1)$. The self- consistent gap equation for the system is found by:

$$\Delta^{(j)} = \frac{V}{2a} \int_{(2n-1)a}^{(2n+1)a} F(x, \Delta) dx,$$

where $F(x)$ is the pair amplitude. We note that the gaps for each superconducting layer are different, and therefore we use the label j to indicate the gap parameter for a particular layer. Now we set up and solve the gap equations

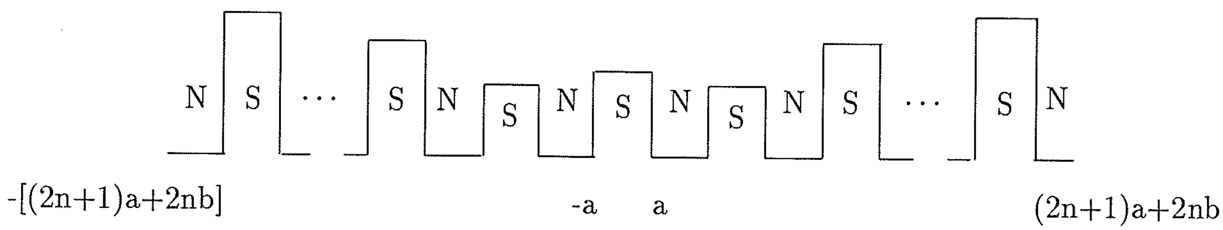

Figure 7.1: Finite Superlattice System

for this geometry using the self-consistency requirement stated before.

1 The Self-Consistent Gap Equation

For the system, we again assume that all physical properties such as the Fermi velocity, the Debye temperature, etc., are the same for both metals, and the transmission and reflection coefficients at the interfaces are unity. The equation of motion for φ is

$$[E + i(q/m)\tau_3 \frac{d}{dx} + \Delta(x)\tau_1]\varphi(E, x) = 0, \tag{1.1}$$

where

$$q = \sqrt{k_F^2 - k_y^2 - k_z^2}$$

and τ_i is the Pauli matrices. The solutions can be labeled by their parity $\pm$, where $\tau_1\varphi_\pm(x) = \pm\varphi_\pm(-x)$. The solutions can thus be split into 2 parity states. Generally, the solutions of the Equation (1.1) in both superconducting regions and normal regions can be written as

$$\begin{aligned}
\varphi_\pm^{(0)}(x) &= A_\pm \begin{pmatrix} 1+\gamma_{(0)} \\ \delta_{(0)} \end{pmatrix} e^{ipx} \pm A_\pm \begin{pmatrix} \delta_{(0)} \\ 1+\gamma_{(0)} \end{pmatrix} e^{-ipx} \\
\varphi_\pm^{(1)}(x) &= B_\pm \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik(x-d)} \pm C_\pm \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik(x-d)} \\
\varphi_\pm^{(2)}(x) &= D_\pm \begin{pmatrix} 1+\gamma_{(1)} \\ \delta_{(1)} \end{pmatrix} e^{ip(x-2d)} \pm E_\pm \begin{pmatrix} \delta_{(1)} \\ 1+\gamma_{(1)} \end{pmatrix} e^{-ip(x-2d)} \\
\varphi_\pm^{(3)}(x) &= F_\pm \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik(x-3d)} \pm G_\pm \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik(x-3d)} \\
\varphi_\pm^{(4)}(x) &= H_\pm \begin{pmatrix} 1+\gamma^{(2)} \\ \delta^{(2)} \end{pmatrix} e^{ip(x-4d)} \pm I_\pm \begin{pmatrix} \delta_{(2)} \\ 1+\gamma_{(2)} \end{pmatrix} e^{-ip(x-4d)} \\
\vdots &= \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
\varphi_\pm^{(10)}(x) &= T_\pm \begin{pmatrix} 1+\gamma_{(5)} \\ \delta_{(5)} \end{pmatrix} e^{ip(x-10d)} \pm U_\pm \begin{pmatrix} \delta_{(5)} \\ 1+\gamma_{(5)} \end{pmatrix} e^{-ip(x-10d)} \\
\varphi_\pm^{(11)}(x) &= V_\pm \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik(x-11d)} \pm W_\pm \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ip(x-11d)} \\
\vdots &= \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
\varphi_\pm^{(n)}(x) &= Y_\pm \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik(x-nd)} \pm Z_\pm \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik(x-nd)},
\end{aligned} \tag{1.2}$$

where $n = 0, 1, 2, 3, 4, \ldots n-1$, $d = a + b$, and

$$p = k\gamma_{(j)} \qquad k = mE/q \qquad \delta_{(j)} = -\Delta^{(j)}/E \qquad \gamma_{(j)} = \sqrt{1-\delta_{(j)}^2}.$$

The solutions for $x < 0$ are obtained by

$$\varphi_\pm(-x) \to \pm\tau_1\varphi_\pm(x).$$

The coefficients in Equation (1.2) are determined by continuity at the interface and the normalization condition. Applying such conditions, the following relations between the coefficients can be obtained:

$$| B_\pm |^2 = | C_\pm |^2,$$

$$| D_\pm |^2 = | E_\pm |^2,$$

$$\vdots$$

and

$$| Y_\pm |^2 = | Z_\pm |^2 .$$

For the last normal layer, we find

$$\begin{aligned} \int_{-\infty}^{\infty} dx \quad & \varphi^*(E', x)\varphi(E, x) = 2\pi\delta(E - E') \\ = \quad & 2\pi\frac{| q |}{m}[| Y_\pm |^2 + | Z_\pm |^2]\delta(E - E') \\ & | Y_\pm |^2 = \frac{m}{2 | q |}. \end{aligned} \tag{1.3}$$

The equation in the superconducting regions can be written in general as

$$\varphi^{(j)}(x) = S_\pm \begin{pmatrix} 1 + \gamma_{(j)} \\ \delta_{(j)} \end{pmatrix} e^{ip(x-2jd)} \pm T_\pm \begin{pmatrix} \delta_{(j)} \\ 1 + \gamma_{(j)} \end{pmatrix} e^{-ip(x-2jd)}, \tag{1.4}$$

where $j = 0, 1, 2, 3, \ldots$ represents the layers from the center to the last film on the right side of the system. The total number of layers of the system then is $N = 2j+1$. The $S_\pm, T_\pm$ in Equation (1.4) are the coefficients for any layer and according to the relation between the coefficients we have $S_\pm = T_\pm^* = s_\pm e^{i(2jpd)}$, with $d = a + b$. In terms of the known last normal metal layer, we have

$$4 \mid S_\pm \mid^2 \{1 \pm \delta_{(j)} \cos(2ka + 4jkd)\} = \mid Y_\pm \mid^2 \pm 8 \mid S_\pm \mid^2 \sin 2ka \sum_{j'}^{N-1} \delta_{(j')} \sin(4kj'd), \tag{1.5}$$

where $j' = j+1, j+2, \ldots, m$ are those layers to the right of the j^{th} layer. In Eq.(1.5), we have kept only terms to the first order in $\delta_{(j)}$. We then have

$$4 \mid S_\pm \mid^2 = \mid Y_\pm \mid^2 = \frac{m}{2 \mid q \mid}, \tag{1.6}$$

and with the gap function given by

$$\Delta^{(j)}(x) = \frac{1}{2a} \int dx F(x), \tag{1.7}$$

where $F(x) = -\langle \varphi^\dagger(x) \varphi(x) \rangle_{12}$, the subscripts indicating the matrix components, we find

$$\Delta^{(j)} = \frac{1}{2a} \int_{(2j-1)a+2jb}^{(2j+1)a+2jb} [\varphi^{(j)\dagger} \tau_1 \varphi^{(j)}] dx = 8 \mid S_\pm \mid^2 [\delta_{(j)} \pm \frac{\sin 2ka}{2ka} \cos(4jkd)]. \tag{1.8}$$

Due to the fact that $\Delta(x)$ is assumed to be small, we can neglect higher order terms in Δ.

The gap function can be obtained by substituting Eq.(1.5) into Eq. (1.8) and using some trigonometric identities. After some manipulation we get

$$\begin{aligned}
\frac{1}{gN(0)} &= \int_0^{\omega_d} \frac{dE}{E} \tanh(\beta E/2) \int_0^{k_F} \frac{dq}{k_F} \{(1 - \frac{\sin 4ka}{4ka}) \\
&+ \frac{\sin 4ka}{8ka} + \frac{\sin 8jkd}{8ka} - \frac{\sin 2(4jkd + 2ka)}{8ka} \\
&+ \frac{2}{\Delta^{(j)}} \frac{\sin^2 2ka}{2ka} \cos(4jkd) \sum_{j'}^{N-1} \Delta^{(j')} \sin(4j'kd)\},
\end{aligned} \tag{1.9}$$

where $N(0) = mk_F/2\pi^2$ is the density of states at the Fermi surface of the normal metal for one spin projection, and g is the coupling constant.

For the single film case, we have $j = 0 = j'$ and $N = 2j + 1 = 1$, and so Equation (1.9) reduces to:

$$\frac{1}{gN(0)} = \int_0^{\omega_d} \frac{dE}{E} \tanh(\beta E/2) \int_0^{k_F} \frac{dq}{k_F}[(1 - \frac{\sin 4ka}{4ka})].$$

This is consistent with the single film calculation given in Chapter 5.

We can now determine some properties of the system by solving this self-consistent gap function.

2 Determination of Some Properties

In this section we solve the self-consistent gap Equation (1.9) and determine some properties of the system. Specifically, we shall calculate the reduced thickness a/a_c at zero temperature, then investigate the reduced transition temperature, and finally we analyze the behavior of the gap parameters at zero temperature.

2.1 Calculation of a/a_c at $T = 0$

One of the properties for such system is the reduced critical width below which superconductivity is destroyed at zero temperature. This width is a function of the normal metal width b and the number of layers. As we shall see the behaviour of this width becomes an important factor in determining the validity of the approximation $\Lambda\Omega_d \gg 1$, which simplifies significantly the calculations. In this section we present the calculation of the reduced dependence of thickness a/a_c at zero temperature.

First let us define a function as

$$I(\omega) = \frac{1}{k_F} \int_0^{\omega} \frac{dE'}{dE'} \int_0^{k_F} dq(1 - \frac{\sin 4ka}{4ka})$$

$$
\begin{aligned}
&+ \frac{\sin 4ka}{8ka} + \frac{\sin 8jkd}{8ka} - \frac{\sin 2(4jkd + 2ka)}{8ka} \\
&+ \frac{2}{\Delta^{(j)}} \frac{\sin^2 2ka}{2ka} \cos(4jkd) \sum_{j'}^{N-1} \Delta^{(j')} \sin(4j'kd),
\end{aligned} \tag{2.10}
$$

so that after integrating (1.9) by parts, the gap function can be rewritten as

$$
\frac{1}{gN(0)} = [I(\omega_d) - \frac{\beta}{2} \int_0^\infty d\omega I(\omega) \cosh^{-2}(\frac{\beta\omega}{2})]. \tag{2.11}
$$

In this equation, the first term $I(\omega_d)$ represents the contribution to the gap function at $T = 0$, with the other term containing the thermal contribution to the system. To calculate the dependence of the thickness at zero temperature, we only need to consider the first term of Eq. (2.11). The function $I(\omega_d)$ is given by

$$
I(\omega_d) = I(\Lambda\Omega_d),
$$

where

$$
\Lambda = 2k_F a, \qquad \Omega_d = \frac{\omega_d}{E_F},
$$

which have been defined in previous Chapters. If we consider the $j = N$ equation in (2.10), we have, with $\Delta^{(j)} \to 0$,

$$
I(x) = \gamma_e + \ln x + J(x), \tag{2.12}
$$

where the function $J(x)$ is defined as follows:

$$
\begin{aligned}
J(x) &= \frac{1}{2} \ln(2\alpha + 1) + \alpha \ln(1 + 1/2\alpha) \\
&+ \frac{1}{2}[\frac{\sin x}{x} - \cos(x) - 2Ci(x) - xSi(x)] \\
&- \frac{1}{2}[\frac{\sin 2x}{2x} - \cos(2x) - 2Ci(2x) - 2xSi(2x)] \\
&- \frac{\alpha}{2}[\frac{\sin 4\alpha x}{4\alpha x} - \cos(4\alpha x) - 2Ci(4\alpha x) - 4\alpha x Si(4\alpha x)] \\
&+ \frac{1}{2}\{\frac{4\alpha + 2}{4}[\frac{\sin(4\alpha + 2)x}{(4\alpha + 2)x} - \cos(4\alpha + 2)x \\
&- 2Ci(4\alpha + 2)x - (4\alpha + 2)xSi(4\alpha + 2)x]\},
\end{aligned} \tag{2.13}
$$

where $\alpha = j(\frac{d}{a}) = j(1 + \frac{b}{a})$ and $Ci(x)$ and $Si(x)$ are the Cosine and Sine integrals. This solution is the exact solution of Eq. (2.10). For large x, the function becomes

$$\lim_{x\to\infty} J(x) \approx \frac{1}{2}\ln(2\alpha+1) + \alpha\ln(1+1/2\alpha) + O(\frac{1}{x^3}). \tag{2.14}$$

For $x \to 0$ the function $I(x)$ can be approximated as

$$\lim_{x\to 0} I(x) \approx \frac{\pi}{4}x(1+2\alpha) + O(x^2). \tag{2.15}$$

Defining the critical thickness for a single superconductor layer, a_c, below which the superconducting state no longer exists at any temperature, $T_c(a_c) = 0$, we have

$$a_c = \frac{1}{\pi k_F}(\frac{T_F}{T_c}), \tag{2.16}$$

where $T_F = E_F/k_B$ is the Fermi temperature. a_c also can be written in terms of the coherence length as

$$a_c \approx 0.882\xi_0.$$

This critical thickness a_c will be used as a length scale, so that the ratio b/a, the width of normal layer and the width of superconductor layer can be written as b/a_c and a/a_c. It is also useful to write $\Lambda\Omega_d$ in terms of a/a_c:

$$\Lambda\Omega_d = \frac{2}{\pi}\frac{\theta_D}{T_c}\frac{a}{a_c}, \tag{2.17}$$

where θ_D is the Debye temperature and T_c is the bulk superconducting transition temperature.

Assuming that $\Lambda_c\Omega_d \gg 1$, with $\Lambda_c = 2k_F a_c$, we then solve

$$\frac{1}{gN(0)} = \gamma_e + \ln(\Lambda_c\Omega_d) \tag{2.18}$$

and

$$\frac{1}{gN(0)} = \gamma_e + \ln(\Lambda\Omega_d) + J(x), \tag{2.19}$$

by which

$$\ln(\frac{a}{a_c}) = -J(x), \tag{2.20}$$

where a/a_c is the reduced critical thickness (i.e., the thickness below which the superconducting layers become normal at $T = 0$). This equation can be solved numerically: note the solution is independent of the material. Figure 7.2 presents the relations between a/a_c and b/a_c for various values of j at zero temperature. As we can see, either b/a_c or j increasing causes a/a_c to decrease. This b/a_c and j dependent reduced critical width will be an important factor in deciding on the validity of the approximation $\Lambda\Omega_d \gg 1$ in future calculations.

2.2 Calculation of $T_c(a, b, j)$

In order to determine the thickness dependence of the reduced critical temperature above which the superconductors become normal, we return to Equation (2.11). At finite temperature, we have to consider the second term of Equation (2.11). With $\Delta^{(j)} \to 0$, (2.11) together with (2.12) gives

$$\ln(\frac{a}{a_c}) = -J(x) + \frac{1}{\tau}\int_0^\infty dx J(x)\cosh^{-2}(\frac{x}{\tau}), \qquad (2.21)$$

where

$$x = \Lambda\Omega_d = 2k_F a(\frac{\omega_d}{E_F}) = \frac{2}{\pi}\frac{a}{a_c}\frac{\omega_d}{T_c}$$

and

$$\tau = \frac{4}{\pi}\frac{a}{a_c}\frac{T}{T_c}.$$

Assuming that $\Lambda\Omega_d \gg 1$, i.e. $x \gg 1$, then the approximation for J(x) given in Equation (2.14) can be used, so that the above equation can be written as

$$\ln(\frac{a}{a_c}) = -[\frac{1}{2}\ln(2\alpha+1) + \alpha\ln(1+1/2\alpha)] + \frac{1}{\tau}\int_0^\infty dx J(x)\cosh^{-2}(\frac{x}{\tau}). \qquad (2.22)$$

After integration of the second term, the equation becomes

$$\ln(\frac{a}{a_c}) = \ln(\frac{\pi\tau}{4}) + \frac{1}{\tau}\int_0^\infty dx G(x)\cosh^{-2}(\frac{x}{\tau}), \qquad (2.23)$$

and using the expression for τ, T_c/T can be obtained as follows:

$$\ln(\frac{T_c}{T}) = \frac{1}{\tau}\int_0^\infty dx G(x)\cosh^{-2}(\frac{x}{\tau}), \qquad (2.24)$$

where the function G(x) is defined as:

$$\begin{aligned} G(x) &= \frac{1}{2}[\frac{\sin x}{x} - \cos(x) - 2Ci(x) - xSi(x)] \\ &- \frac{1}{2}[\frac{\sin 2x}{2x} - \cos(2x) - 2Ci(2x) - 2xSi(2x)] \end{aligned}$$

$$
\begin{aligned}
&- \frac{\alpha}{2}[\frac{\sin 4\alpha x}{4\alpha x} - \cos(4\alpha x) - 2Ci(4\alpha x) - 4\alpha x Si(4\alpha x)] \\
&+ \frac{1}{2}\{\frac{4\alpha+2}{4}[\frac{\sin(4\alpha+2)x}{(4\alpha+2)x} - \cos(4\alpha+2)x \\
&- 2Ci(4\alpha+2)x - (4\alpha+2)xSi(4\alpha+2)x]\}. \qquad (2.25)
\end{aligned}
$$

Integrating this equation, we obtain T/T_c as function of j, b/a_c, and a/a_c as

$$
\begin{aligned}
\ln(\frac{T}{T_c}) = -\frac{3\pi}{16\tau} &- \frac{1}{2}\int_1^\infty dy(1-\frac{1}{y^2})\ln\tanh(\frac{\pi\tau y}{4}) \\
&+ \frac{1}{4}\int_1^\infty dy(1-\frac{1}{y^2})\ln\tanh(\frac{\pi\tau y}{2}) \\
&+ \frac{\alpha}{2}\int_1^\infty dy(1-\frac{1}{y^2})\ln\tanh(\pi\tau\alpha y) \\
&- \frac{4\alpha+2}{8}\int_1^\infty dy(1-\frac{1}{y^2})\ln\tanh[\frac{\pi\tau y}{4}(4\alpha+2)]. \qquad (2.26)
\end{aligned}
$$

The detailed evaluation of the above expression can be found in Appendix B. Numerically evaluating this equation gives results for values of T/T_c vs. a/a_c as b/a_c and j vary. Figures 7.3 and 7.4 show typical curves of T/T_c for various b/a_c and various layers. From both curves, we note that as b/a_c and j increase a/a_c decreases as $T \to 0$. This behavior is unusual , as we expect that for large b the superconducting layers would decouple and hence reduce to the single layer case, for which we expect $a = a_c$. Note also that for $T/T_c \geq 0.3$ the result approaches the bulk limit for all b/a_c and j values, as expected.

2.3 The Behavior of The Energy Gaps

We now turn our attention to the behavior of the gap parameters. In particular, we consider zero temperature and determine the thickness dependence of the gap parameter ratios

$$\frac{\Delta^{(j)}}{\Delta^{(0)}} \quad and \quad \frac{\Delta^{(j)}}{\Delta^{(j-1)}}.$$

This is of interest because the results can be used to examine the reasonability of the method. In principle, the gap parameter $\Delta(x) = VF(x)$ is spatially dependent, where $F(x) = -\langle\psi_\uparrow(x)\psi_\downarrow(x)\rangle$ is the pair amplitude, $\psi_\uparrow(x)$ and $\psi_\downarrow(x)$ are the bounded pair electron wave. By the proximity effect, the leaked electron pairs could interact with other electron pairs which leak from other superconducting regions, and so in the central regions of the system, the electron-electron coupling is expected to be stronger than in those regions away from the center. From this we expect the gaps at the central regions to be larger than in the other regions, and subsequently decrease away from the central layer.

To calculate this behavior, we go back to Equation (1.9) and take into account the terms involving the gap parameters:

$$\int dE \int dk \sum_{j'}^{N-1} 2\frac{\Delta^{(j')}}{\Delta^{(j)}}\frac{\sin y}{y}\cos(2\alpha y)\sin(2\beta y), \tag{2.27}$$

where $\beta = j'\frac{d}{a}$, $\alpha = j\frac{d}{a}$ and $y = 2ka = 2mEa/q$. By using trigonometric identities and integrating the function, we obtain

$$\sum_{j'}^{N-1} 2\frac{\Delta^{(j')}}{\Delta^{(j)}}\Gamma(a,b,j,j'), \tag{2.28}$$

where Γ is defined as follows:

$$\Gamma(x) \quad = \quad -\frac{\mu}{4}[\frac{\sin(2\mu x)}{2\mu x} - \cos(2\mu x) - 2Ci(2\mu x) - Si(2\mu x)]$$

$$
\begin{aligned}
- & \frac{\nu}{4}[\frac{\sin(2\nu x)}{2\nu x} - \cos(2\nu x) - 2Ci(2\nu x) - Si(2\nu x)] \\
+ & \frac{\mu+1}{8}\{\frac{\sin 2(\mu+1)x}{2(\mu+1)x} - \cos 2(\mu+1)x - 2Ci[2(\mu+1)x] - Si[2(\mu+1)x]\} \\
+ & \frac{\mu-1}{8}\{\frac{\sin 2(\mu-1)x}{2(\mu-1)x} - \cos 2(\mu-1)x - 2Ci[2(\mu-1)x] - Si[2(\mu-1)x]\} \\
+ & \frac{\nu+1}{8}\{\frac{\sin 2(\nu+1)x}{2(\nu+1)x} - \cos 2(\nu+1)x - 2Ci[2(\nu+1)x] - Si[2(\nu+1)x]\} \\
+ & \frac{\nu-1}{8}\{\frac{\sin 2(\nu-1)x}{2(\nu-1)x} - \cos 2(\nu-1)x - 2Ci[2(\nu-1)x] - Si[2(\nu-1)x]\} \\
+ & [\frac{\mu}{4}\ln(1-\frac{1}{\mu^2}) + \frac{\nu}{4}\ln(1-\frac{1}{\nu^2}) + \frac{1}{4}\ln(\frac{\mu+1}{\mu-1}) + \frac{1}{4}\ln(\frac{\nu+1}{\nu-1})], \qquad (2.29)
\end{aligned}
$$

where $\mu = \beta + \alpha = (j' + j)d/a$ and $\nu = \beta - \alpha = (j' - j)d/a$. The above equation is the exact solution. For large x, the function can be written as

$$\lim_{x\to\infty} \Gamma = [\frac{\mu}{4}\ln(1-\frac{1}{\mu^2}) + \frac{\nu}{4}\ln(1-\frac{1}{\nu^2}) + \frac{1}{4}\ln(\frac{\mu+1}{\mu-1}) + \frac{1}{4}\ln(\frac{\nu+1}{\nu-1})]. \qquad (2.30)$$

Eq.(1.9) then becomes

$$\frac{1}{gN(0)} = \gamma_e + \ln x + J(x) + \sum_{j'}^{N-1} \frac{2\Delta^{(j')}}{\Delta^{(j)}}\Gamma(x'), \qquad (2.31)$$

where $J(x)$ is given by (2.14) for $\Lambda\Omega_d \gg 1$. For a given j, the above equation generates j equations, and numerically solving these equations gives the gap behavior. Two ratios of interest, $\Delta^{(j)}/\Delta^{(0)}$ and $\Delta^{(j)}/\Delta^{(j-1)}$, are presented from Figures 7.5 to 7.14 for different values of b/a_c and various values of j.

Note that for the case of $b/a_c = 0.01$, $j = 20$, the results are as expected, which indicates the method in this range provides reasonable results. For the cases of $b/a_c = 0.2$, $j = 20$, and $b/a_c = 0.2$, $j = 5$, the ratio $\Delta^{(j)}/\Delta^{(j-1)}$ gives the expected behavior, but $\Delta^{(j)}/\Delta^{(0)}$ does not. For the ranges $b/a_c = 0.3$, $j =$ 20, and $b/a_c = 0.5$, $j = 10$, both configurations gives unexpected behaviour and thus indicate the method in this range does not give reasonable results.

In general, we find that for $j(b/a_c) \leq 4$ the calculation gives reasonable behaviour that qualitatively can be trusted. This implies that for small b/a_c, j can be large, or for large b/a_c, j must be small in order to keep the condition $b/a_c < 4$. One can note that for large j with $b/a_c \leq 0.05$ the results agrees closely with the superlattice results, and also for small b/a_c as j increases the gap functions remain constant until one gets near the edge; such behaviour is what is expected for an infinite superlattice system.

3 Comparison and Discussion

The single film and the superconducting superlattice cases have been compared with other approaches [22, 36]; the comparison, in all cases, gives a good qualitative agreement, but quantitatively differences exist. Even this qualitative agreement is somewhat surprising, as in this approach we assume clean materials with ideal interface, while others, e.g., the McMillan model, assume dirty materials ($l \ll \xi(T)$) with a tunneling interface. In a sense, then, it may be possible to include dirt and reflecting interfaces in this approach by a simple reinterpretation of the parameter a_c, which has been suggested by the good agreement of the step function approximation with more realistic pair potentials in the context of the quasiclassical approximation [41].

For the finite superlattice case, we would expect that as b/a_c increases, the results of T/T_c should be close to the single layer case; i.e., for a large separation of the superconducting layers, each of the layers in the system could be treated as a single layer. However, the results show that as b/a_c increases T/T_c decreases as $T \to 0$, away from the single layer's case, but as $T \to T_c$ the results agree better in all cases. This unexpected behavior as $T \approx 0$ may be explained by considering the assumption $\Lambda\Omega_d \gg 1$. This assumption was made for simplicity, as the equations in this limit are easier to solve, and also because the corrections to this assumption go like $1/(\Lambda\Omega_d)^3$, and $\Lambda\Omega_d \sim \frac{a}{a_c}\frac{\theta_D}{T_c}$ and $\frac{\theta_D}{T_c} \gg 1$. We then solved the equations and find the assumption is valid except for $j(b/a_c) > 4$. Thus, for consistency a/a_c cannot be too small, as otherwise $\Lambda\Omega_d$ will not be large. According to the calculation of a/a_c from Equation (2.16), when b/a_c and j increase a/a_c decreases. For those values of j and b/a_c for which $\Lambda\Omega_d$ was not found to be large, one should go back to the original equations and solve them not assuming $\Lambda\Omega_d \gg 1$. This was done, but the results differed little with the results presented in the graphs except in extreme cases for which $a/a_c \leq 0.001$. This indicates, therefore, a breakdown in the approximations used to derive the original equations, the most likely one being the assumption of a spatially constant gap function.

This view is supported by the fact that most of the unexpected behavior is near $T = 0$, but for $T \rightarrow T_c$ the right limit is reached for all cases. Recall that a central assumption of the approach is that the assumed and calculated pair potentials nearly coincide. The validity of this assumption has been checked in the single layer's case [22], and agreement between the assumed and calculated pair potential was good for $T \rightarrow T_c$ but not great for $T \rightarrow 0$. This indicates the method is more self consistent for $T \rightarrow T_c$ than for $T \rightarrow 0$. Therefore it would be useful to calculate the gap parameters for finite temperature to see if similar conclusions can be drawn.

Another comparison that can be made is the infinite superlattice with a single layer, which is shown in Figure 7.12. The results are reasonable: when b/a_c increases, they approach the single layer situation, which is expected.

4 Conclusions

We presented a method for the self-consistent solution of the Bogoliubov equations for various systems for which the proximity effect is important. For these different geometries we studied solutions of the gap equations which are obtained from the consistency condition imposed on the pair amplitude. This can be used to study the reduced critical temperature in the various systems

In general, the results obtained qualitatively agree with other techniques which have been employed for the proximity effect. Such an agreement suggests that the approach and the assumptions contained in the method are physically reasonable. The central assumption of the method is that the spatial dependence of the electron pair amplitude in the superconducting regions is small and can be treated as a constant to a good approximation. Such an assumption has been checked in the single layer case, and we used the assumption in an infinite and a finite superlattice systems. The results indicate that the assumption is valid except for a finite superlattice system with large j and b/a_c. ($j(b/a_c) > 4$)

Several results obtained by the procedure can be summarized as follows.

(1). In the single film case, there exists a critical value $a_c \approx 0.882\xi_0$ below which superconductivity cannot be maintained at any temperature. The dependence of this critical thickness at zero temperature for the finite superlattice system has been found, and shows that a/a_c decreases as the normal layer's width increases and as the number of layers increases.

(2). An infinite superconducting superlattice system was shown to follow in the context of this method as the limit of a finite system.

(3). The dependence of transition temperature $T(a, b, j)$ for a finite superlattice system has been studied. The results show that near $T \to T_c$ the right limit is reached for all cases, but unexpected results appear for small T. Such behavior indicates that the assumed and calculated pair potential are nearly self-consistent for $T \to T_c$, but near $T = 0$ this assumption starts to break down.

(4). The thickness and the layers dependence of the gap parameter for finite superlattice system at zero temperature,

$$\frac{\Delta^{(j)}}{\Delta^{(0)}} \quad \frac{\Delta^{(j)}}{\Delta^{(j-1)}},$$

has been studied. The numerical evaluation suggests that the method is reasonable for ranges of j and b/a_c for which $j(b/a_c) \leq 4$

One could mention here again that all the results obtained in this approach are independent of the material with $\Lambda\Omega_d \gg 1$.

The results obtained for the various systems by this approach have also been compared with other techniques. Generally the approach qualitatively agrees with other approaches involving realistic treatments taking into account impurities and moderate deviations from our assumptions of the identical physical properties, e.g.. electron mass, etc. This suggests the method and the assumptions are relatively reasonable. For the finite superlattice system, under the assumption $\Lambda\Omega_d \gg 1$, the calculation gives reasonable solutions at the lower range of the thickness of the normal layer, b/a_c, but for large b the calculation does not provide reasonable results. However, for large b/a_c we can treat each layer of the system as an independent single superconductor layer, so that the treatment of a single layer can apply to each layer of the system separately. In practice, therefore, such approximate calculations for a finite superlattice seems to be a reasonable treatment.

In any case, the procedures in this method provide a mathematically well-defined approach for determining properties of superlattice systems by using only the parameters contained in the BCS theory of bulk superconductors, and it is hoped also provides qualitative picture of the real situation. Therefore, the method generally achieves the goals that many properties of different geometrical systems difficult to obtain in more involved approaches can be calculated in this method by using a straightforward extension of the BCS theory. Other interesting extensions, such as including magnetic order in the normal metal, could also be considered for these systems by this method.

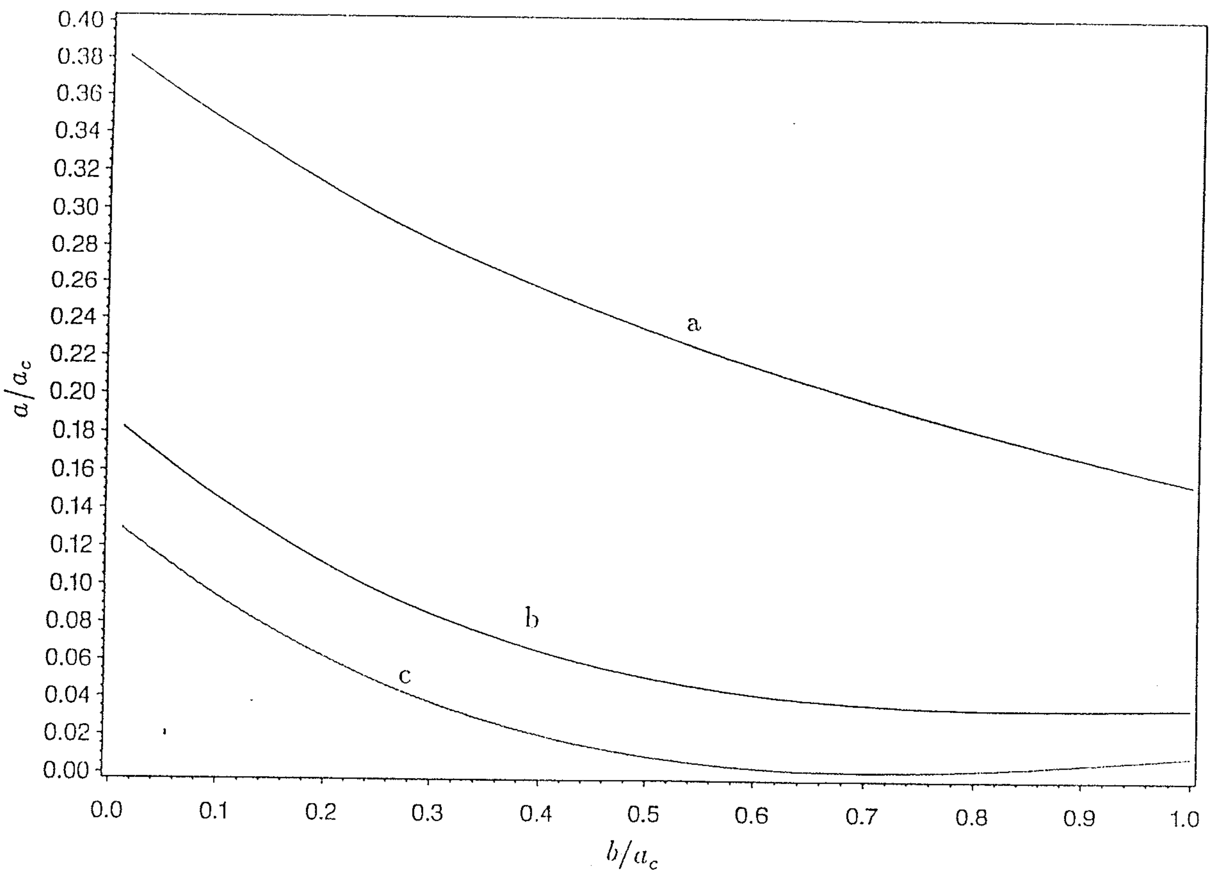

Figure 7.2: The relationship of the reduced critical width a/a_c and b/a_c, for various j system, (a) $j = 2$, (b) $j = 5$, (c) $j = 15$.

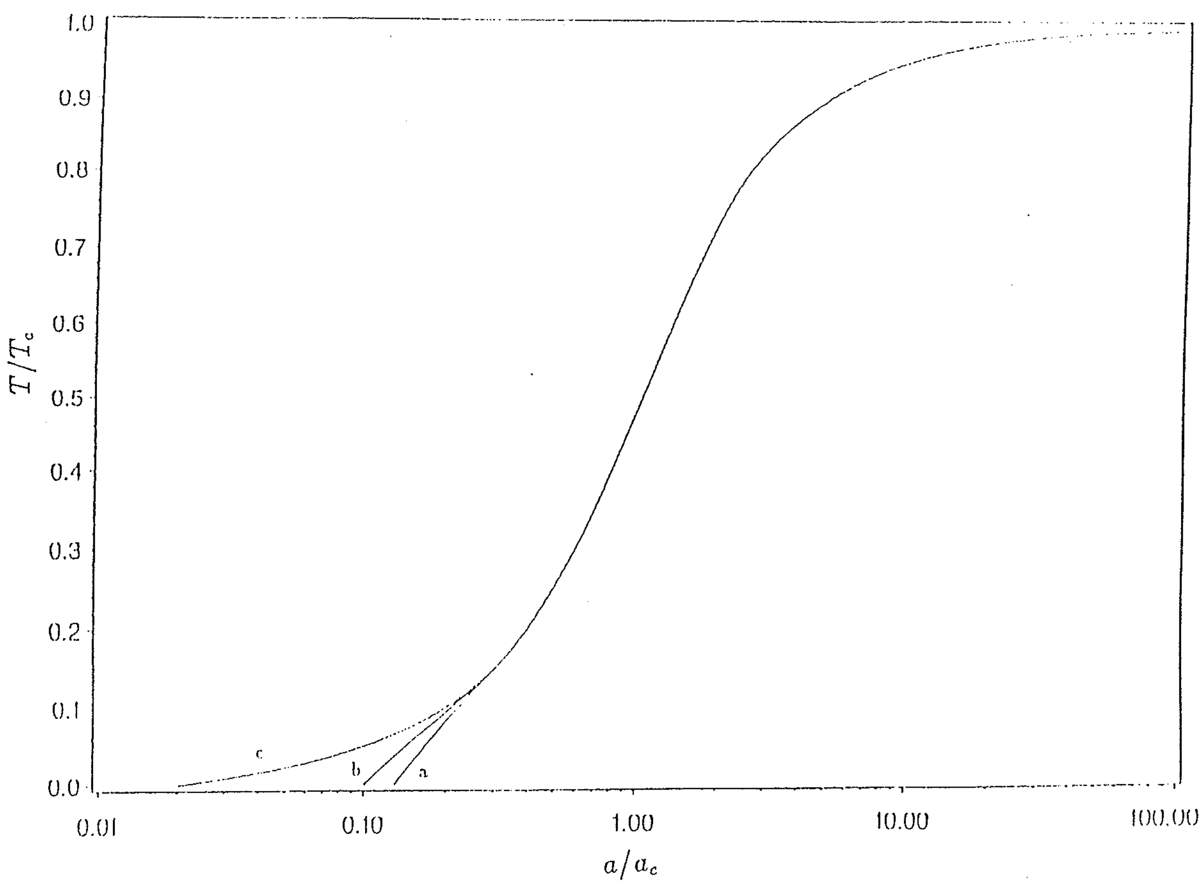

Figure 7.3: The dependence of the reduced temperature $T(a,b,j)/T_c$ on the thickness a/a_c. (a) $b/a_c = 0.01$, (b) $b/a_c = 0.1$, (c) $b/a_c = 1.0$, for 10 layers

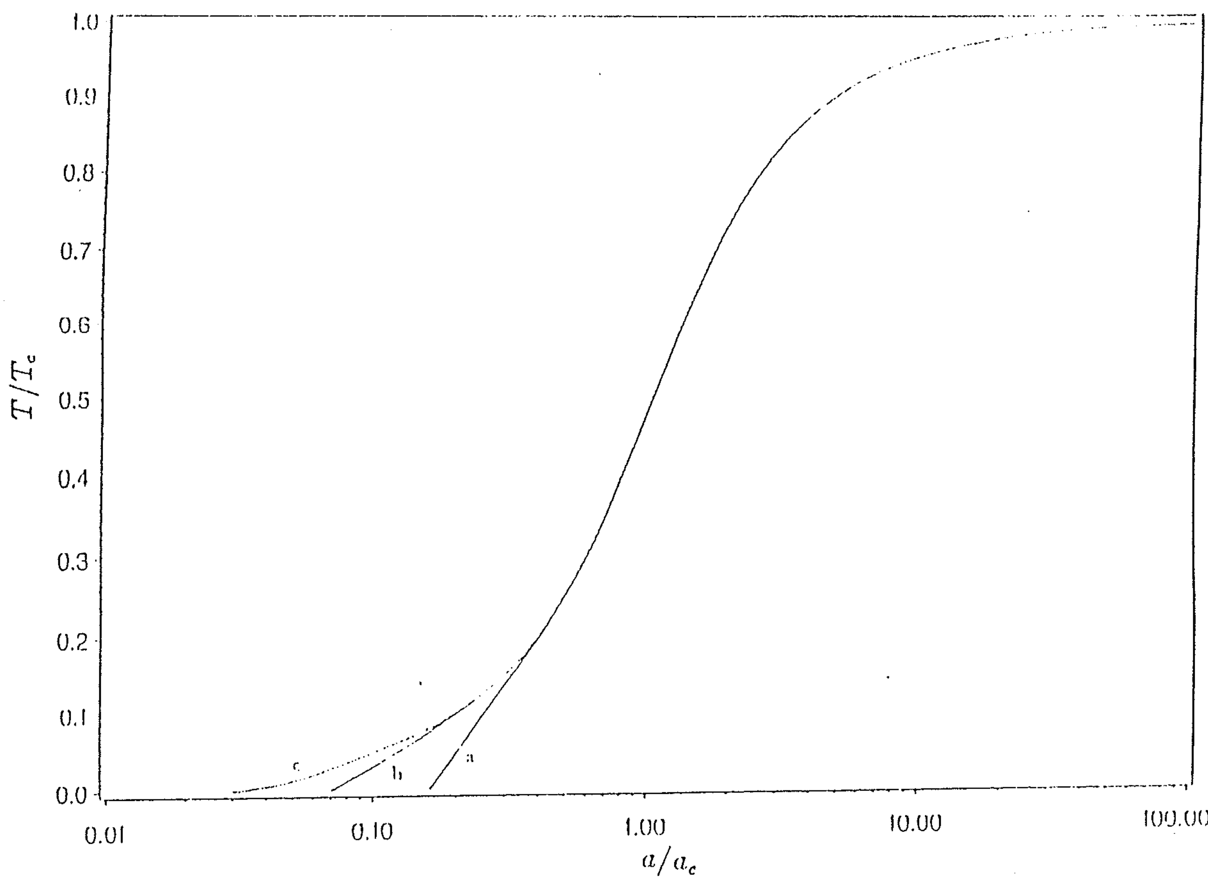

Figure 7.4: The dependence of the reduced temperature $T(a,b,j)/T_c$ on the thickness a/a_c. (a) j=5 (b) j=15 (c) j=35 for $b/a_c = 0.1$

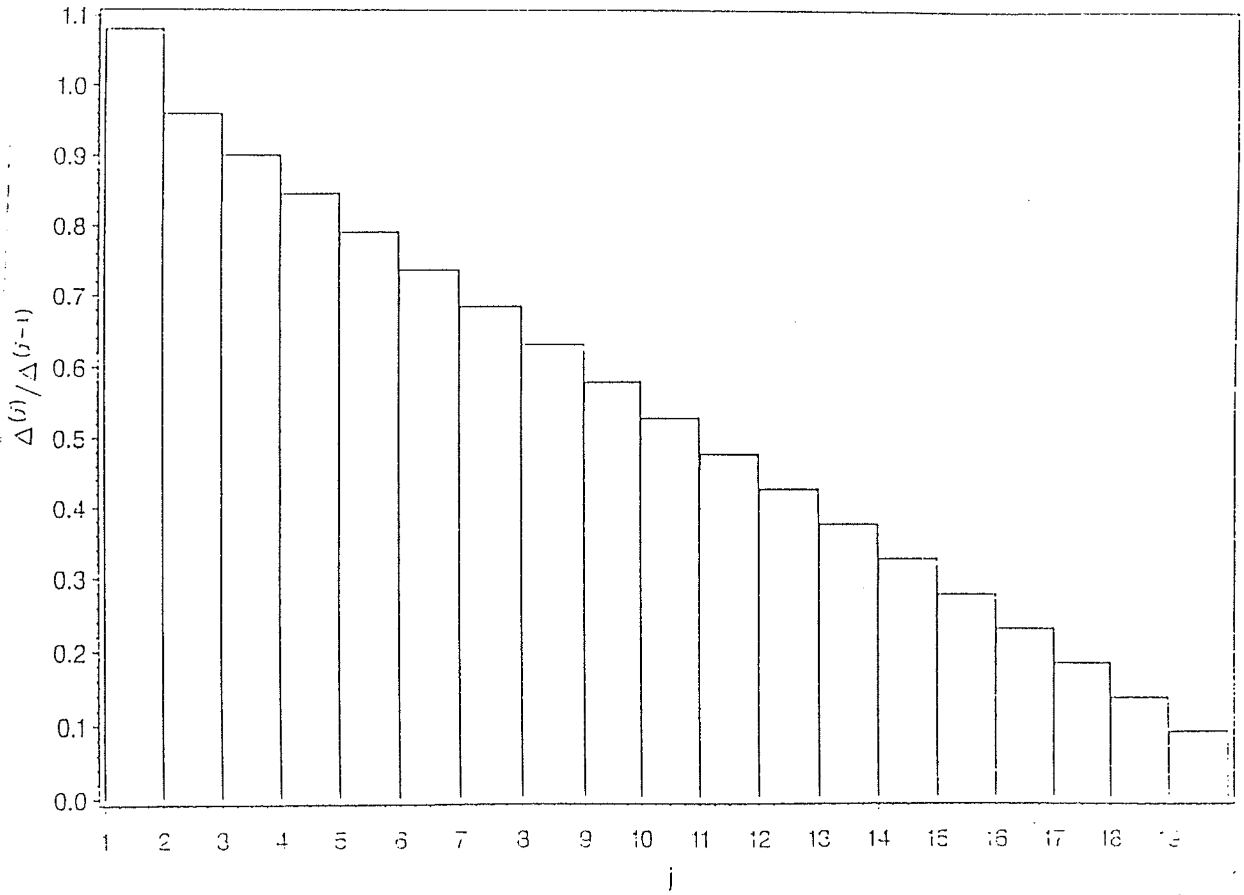

Figure 7.5: The gap parameter ratio $\Delta^{(j)}/\Delta^{(j-1)}$, for $b/a_c = 0.01$, $j = 20$.

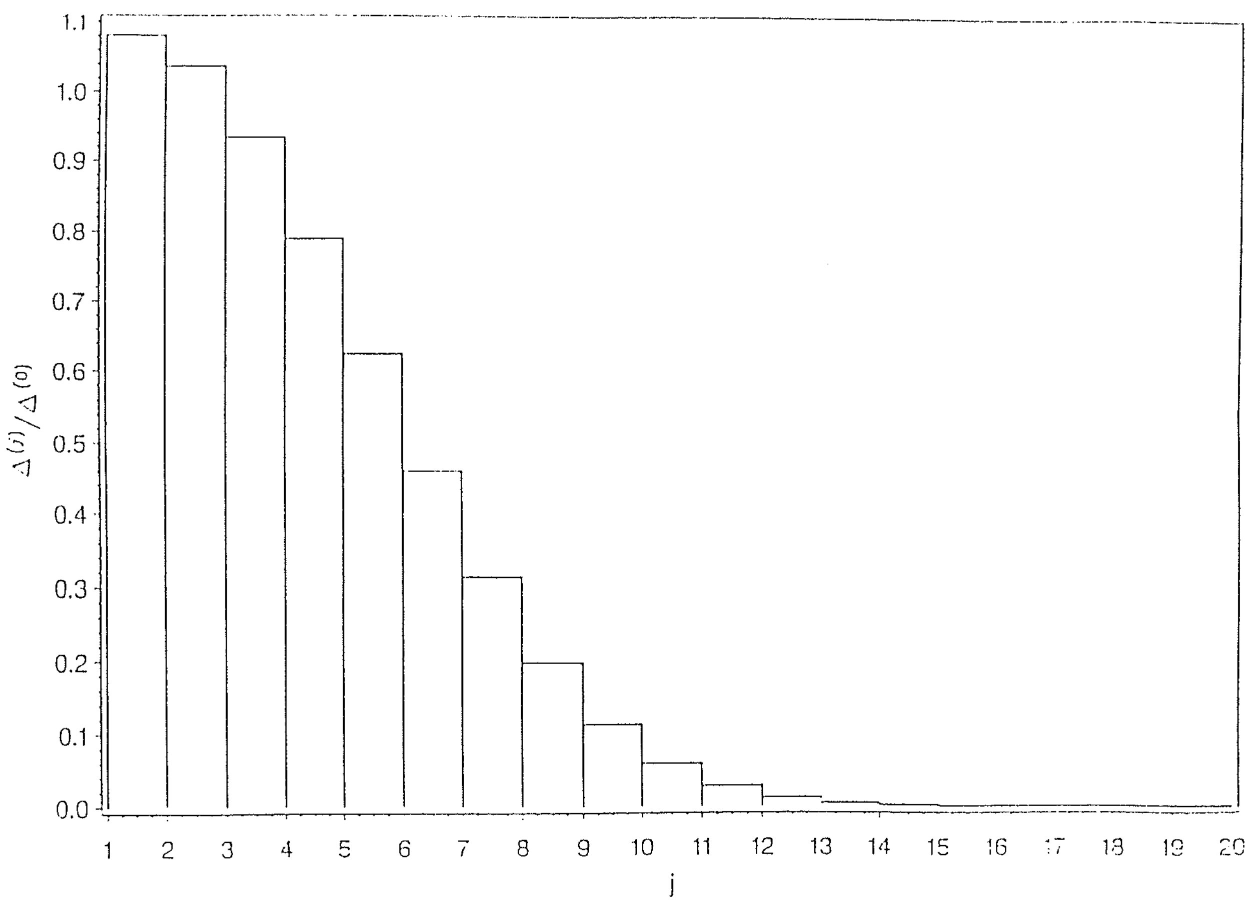

Figure 7.6: The gap parameter ratio $\Delta^{(j)}/\Delta^{(0)}$, for $b/a_c = 0.01$, $j = 20$.

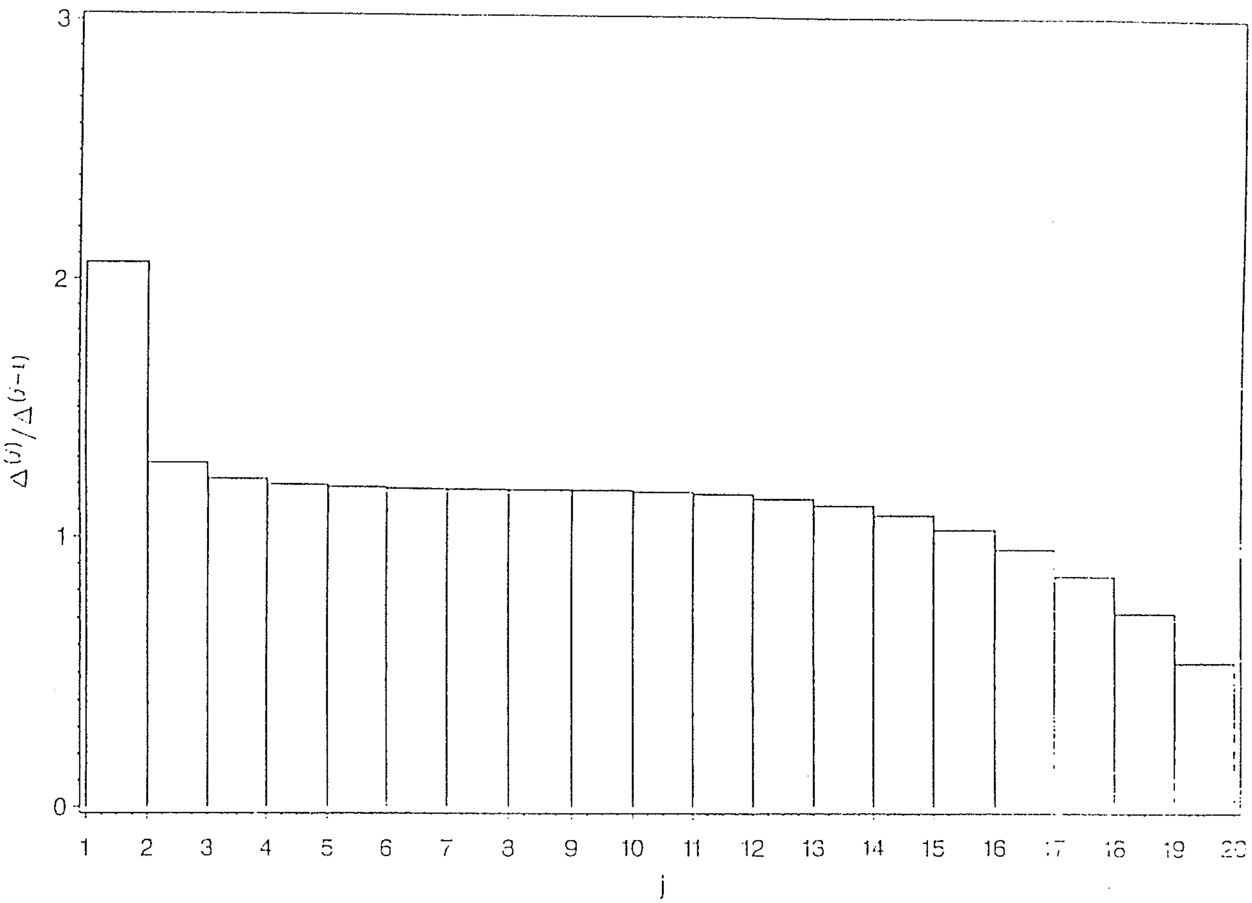

Figure 7.7: The gap parameter ratio $\Delta^{(j)}/\Delta^{(j-1)}$. for $b/a_c = 0.2$, $j = 20$

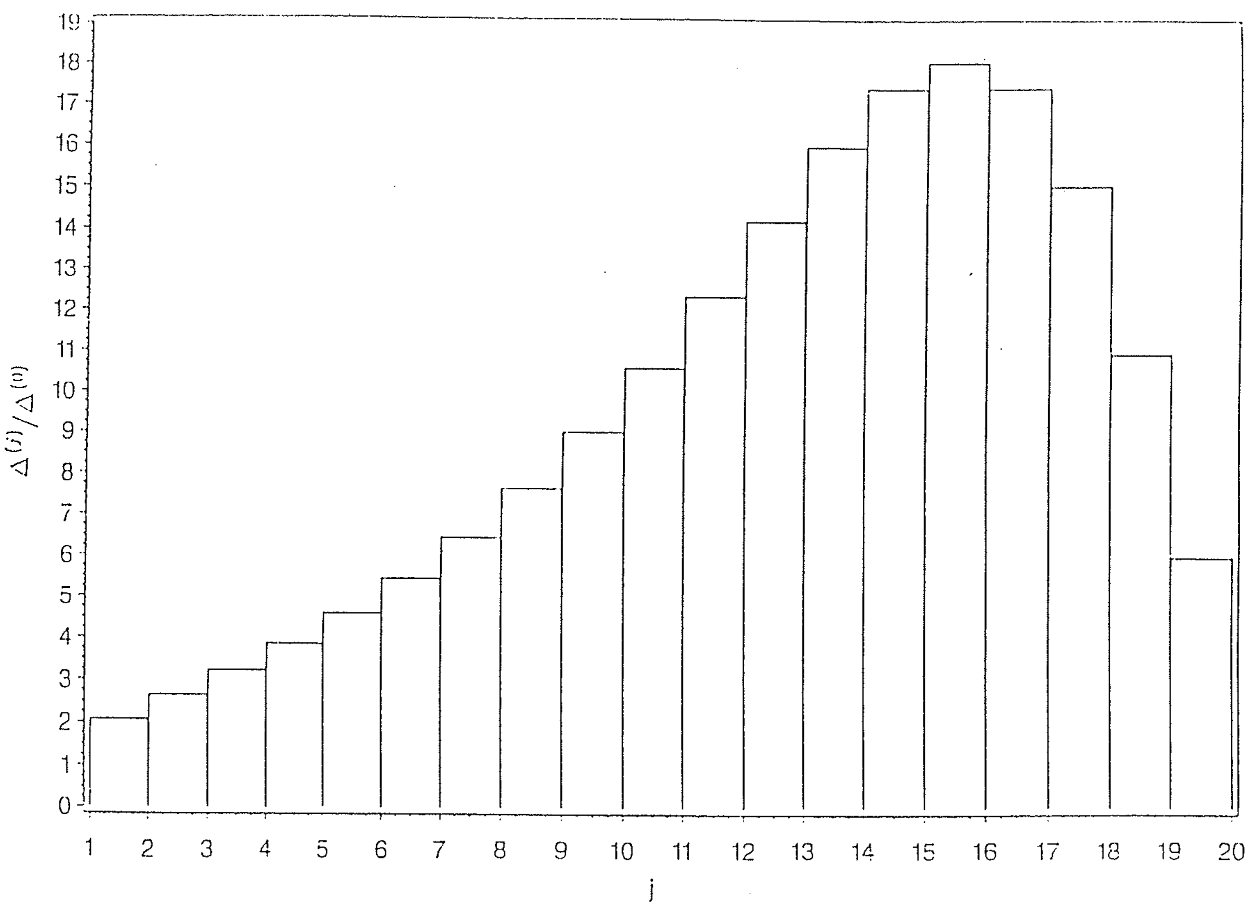

Figure 7.8: The gap parameter ratio $\Delta^{(j)}/\Delta^{(0)}$. For $b/a_c = 0.2$, $j = 20$.

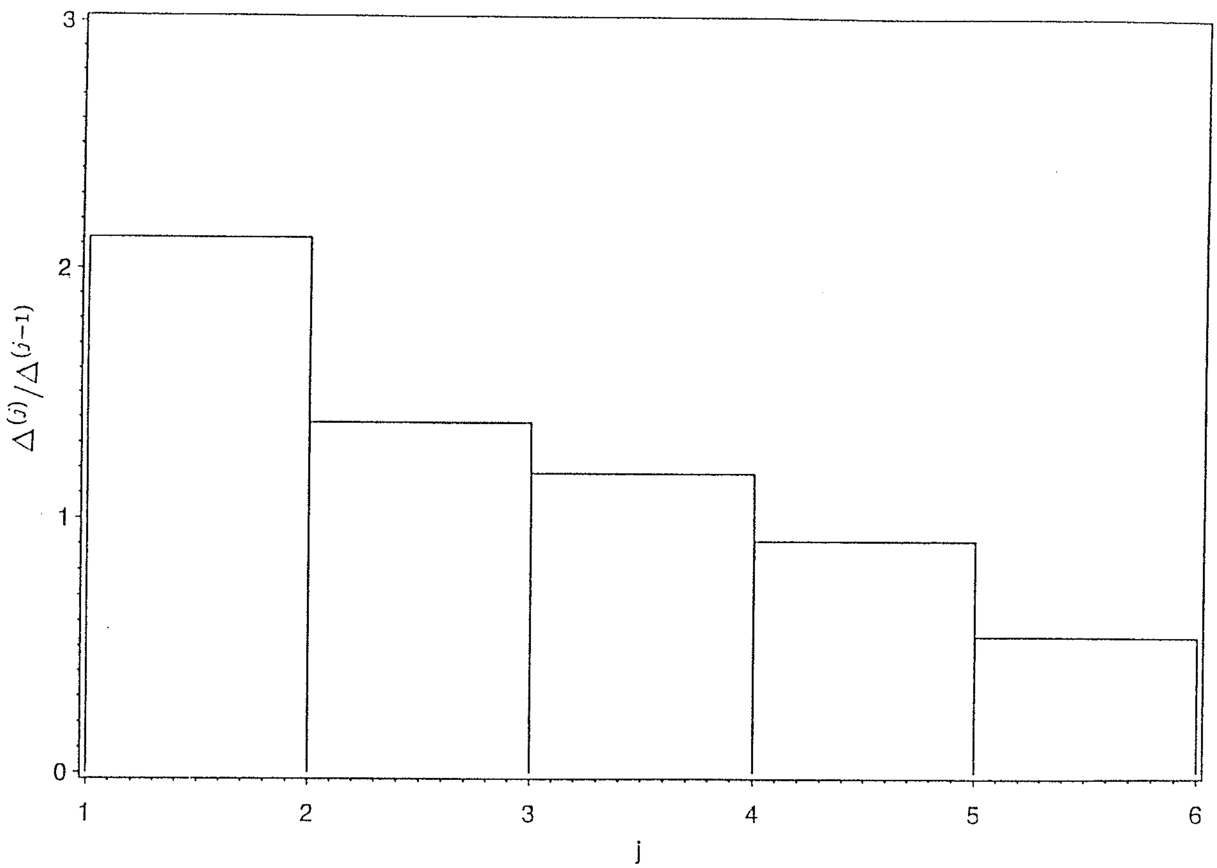

Figure 7.9: The gap parameter ratio $\Delta^{(j)}/\Delta^{(j-1)}$. For $b/a_c = 0.2$ $j = 5$.

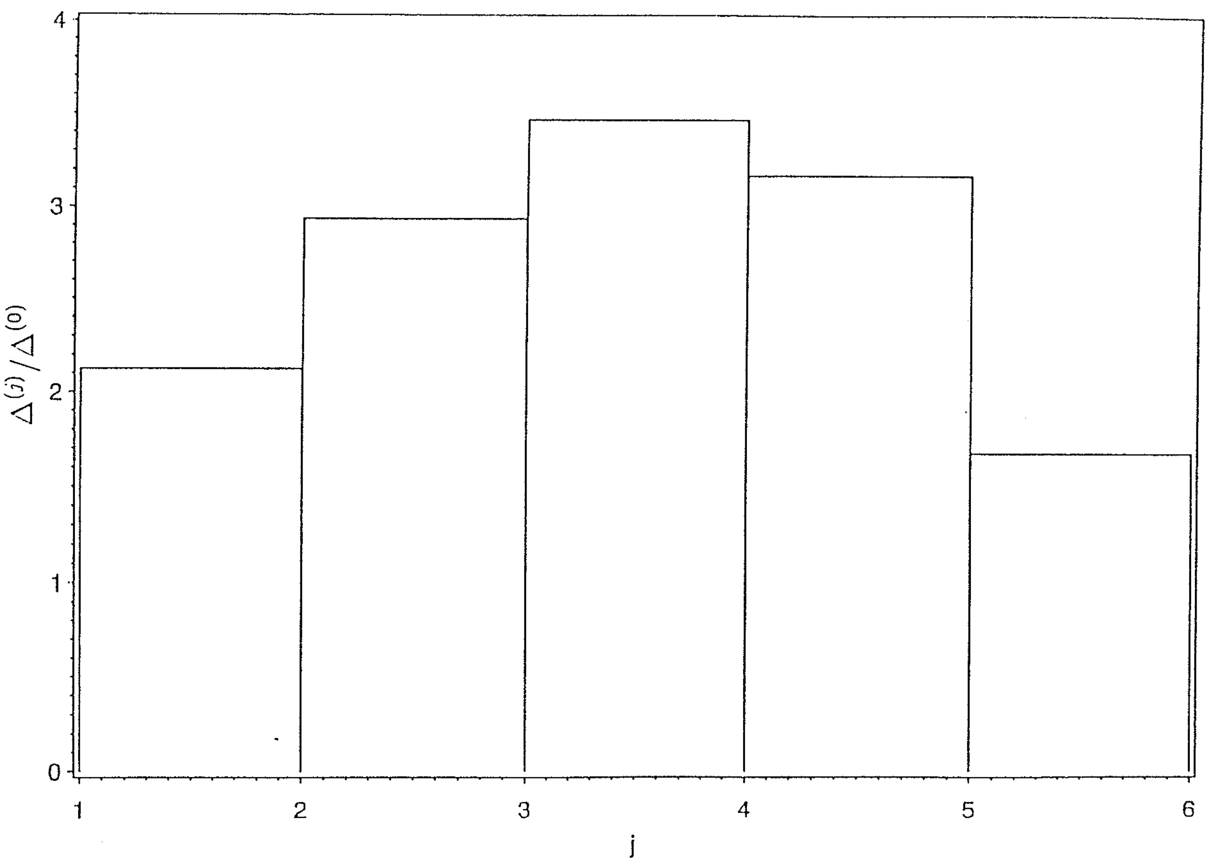

Figure 7.10: The gap parameter $\Delta^{(j)}/\Delta^{(0)}$. For $b/a_c = 0.2$, $j = 5$.

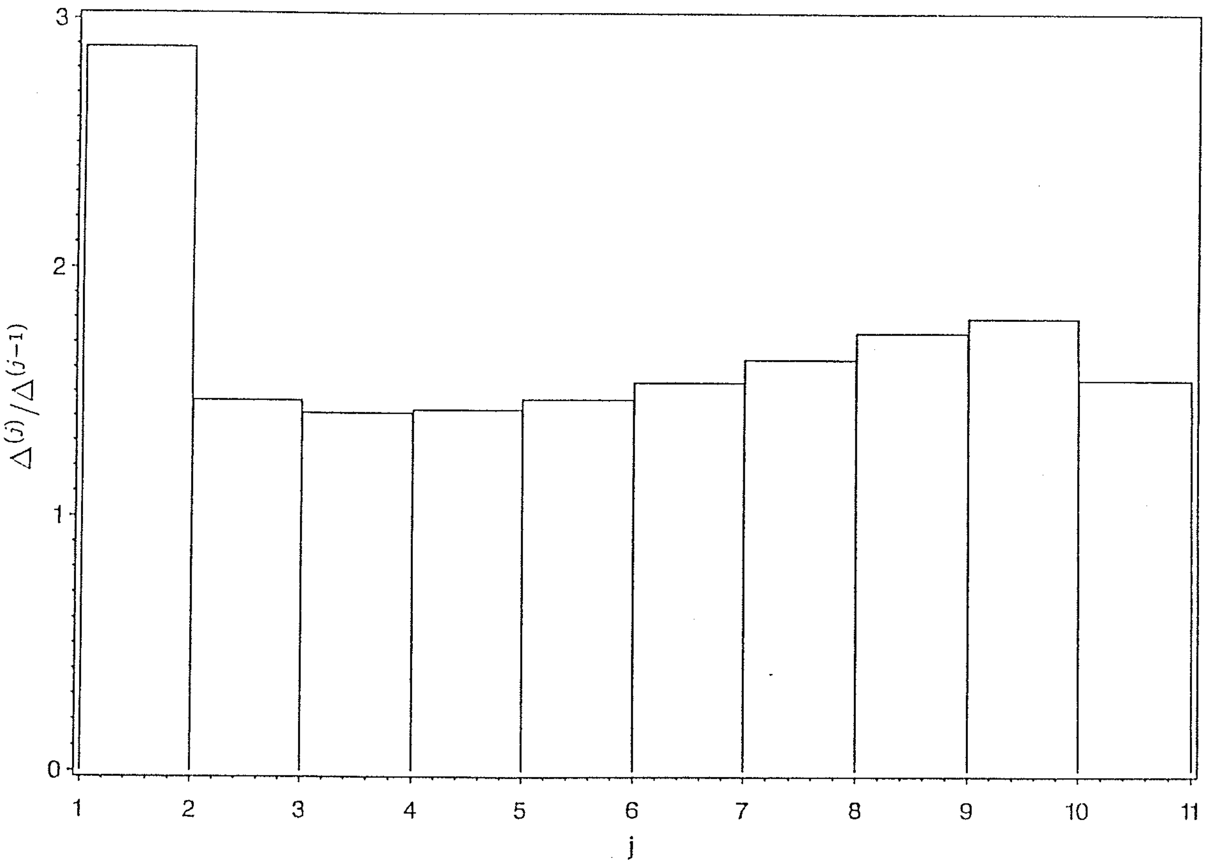

Figure 7.11: The gap parameter $\Delta^{(j)}/\Delta^{(j-1)}$. For $b/a_c = 0.5$, $j = 10$.

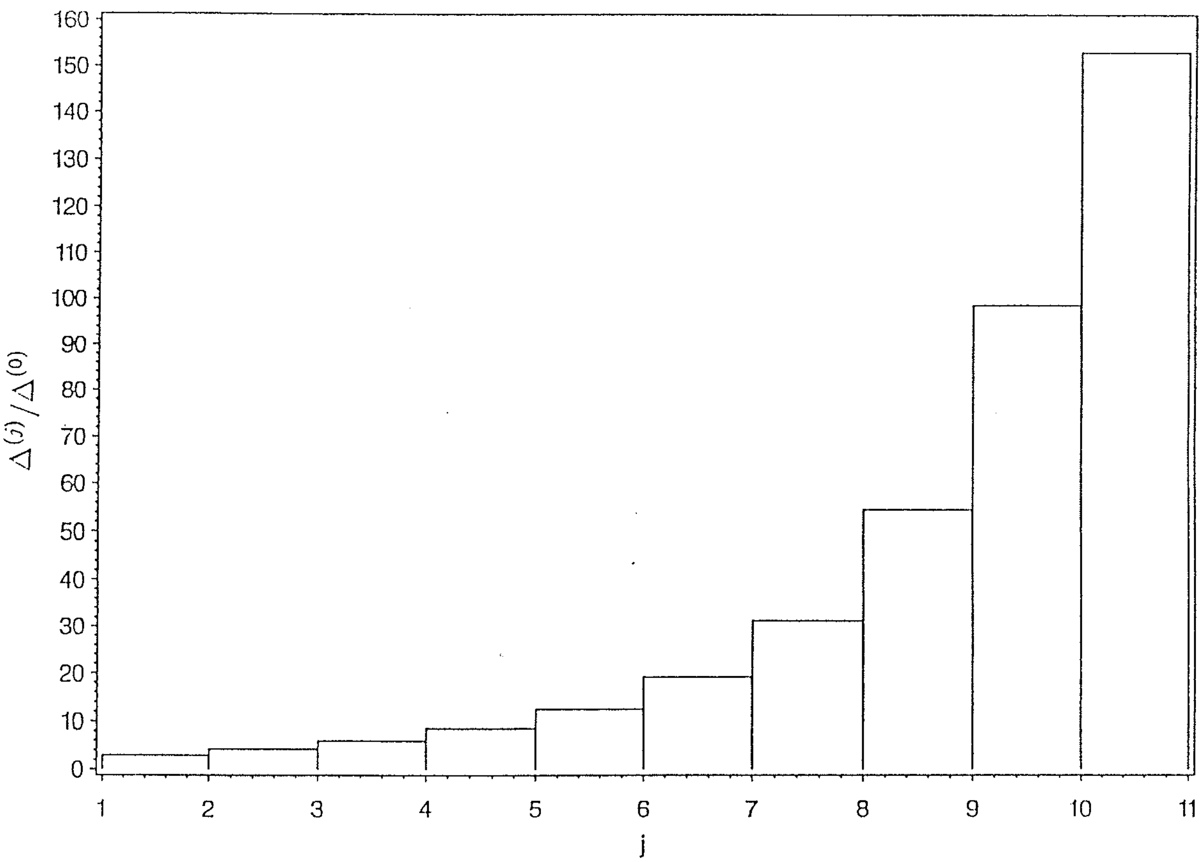

Figure 7.12: The gap parameter $\Delta^{(j)}/\Delta^{(0)}$. For $b/a_c = 0.5$, $j = 10$.

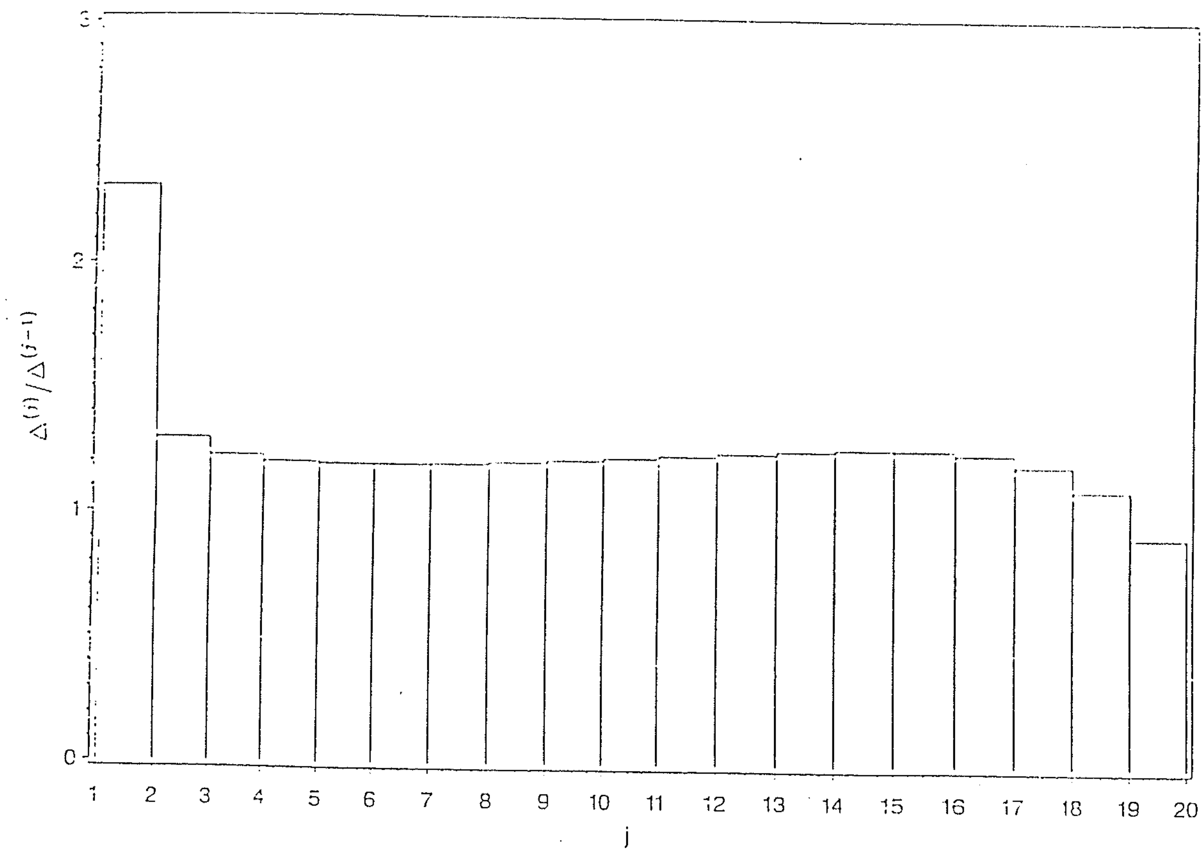

Figure 7.13: The gap parameter $\Delta^{(j)}/\Delta^{(j-1)}$. For $b/a_c = 0.3$, $j = 20$.

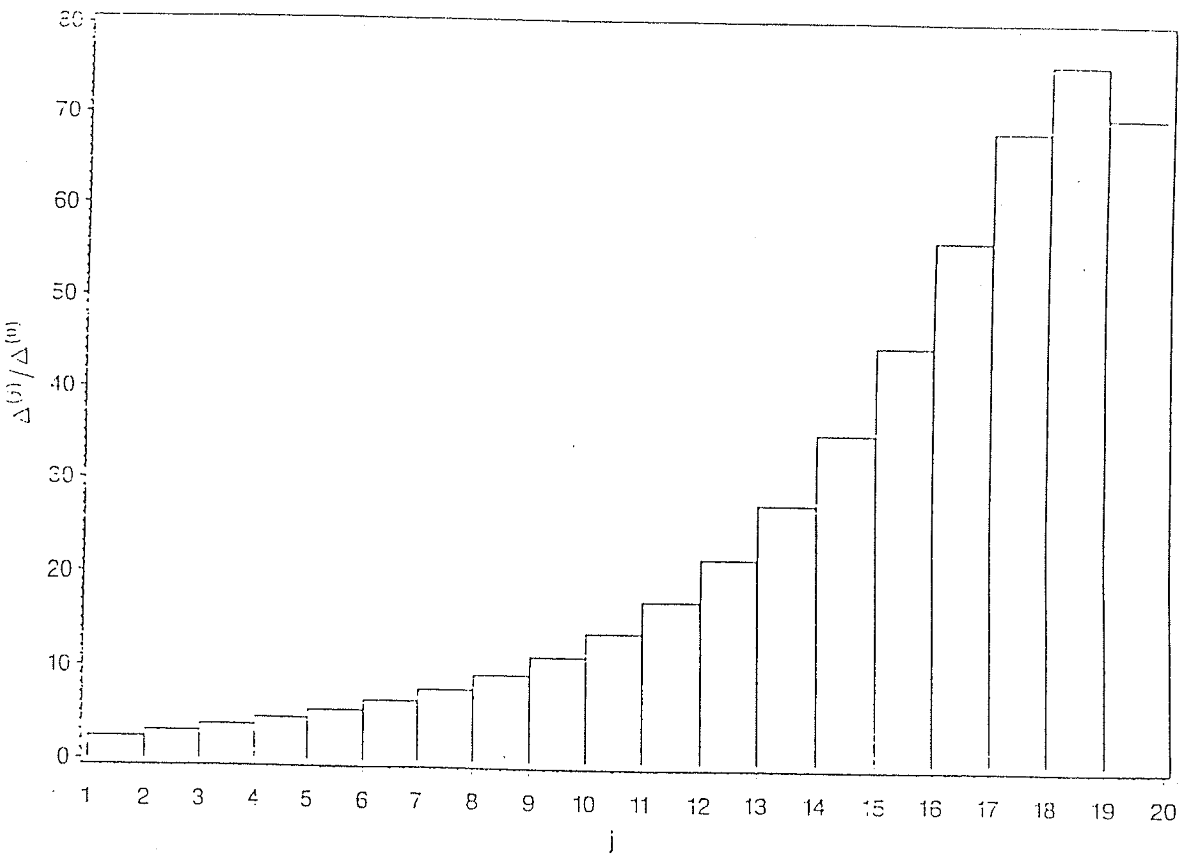

Figure 7.14: The gap parameter $\Delta^{(j)}/\Delta^{(0)}$. For $b/a_c = 0.3$, $j = 20$.

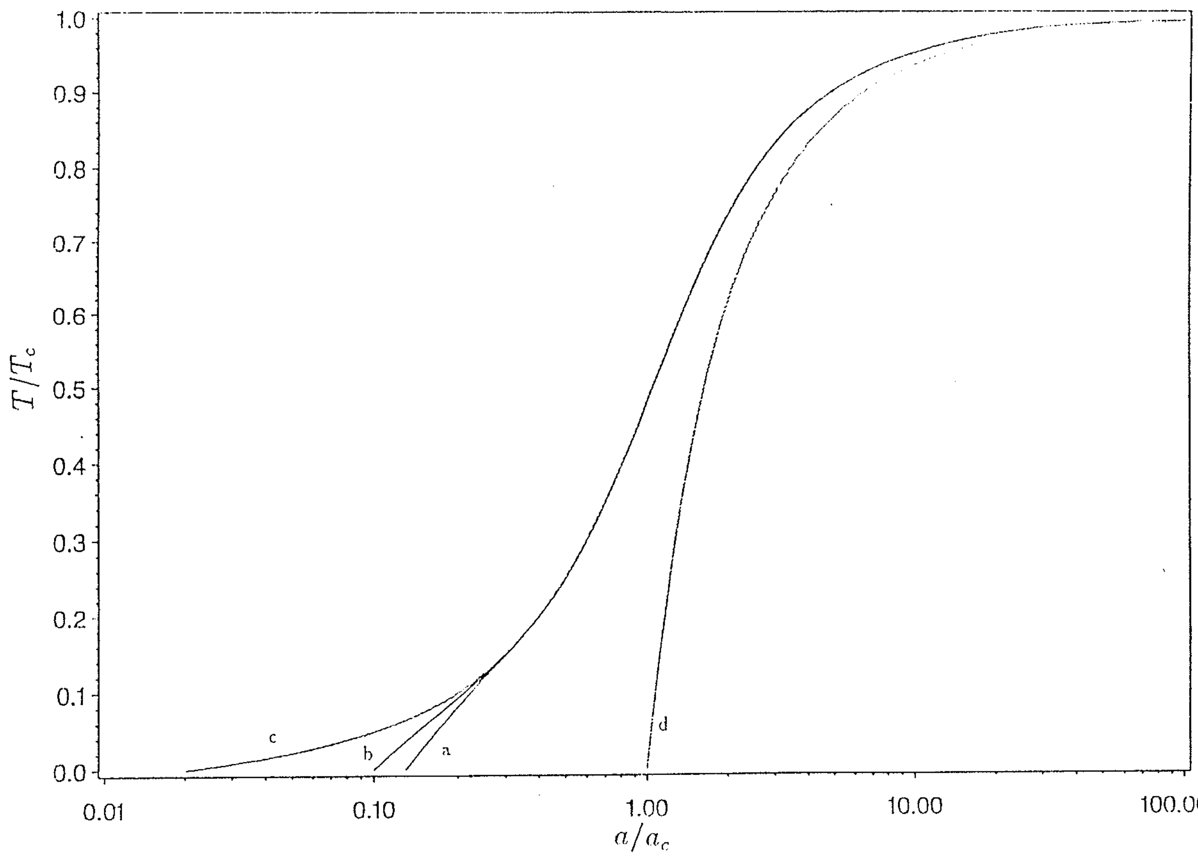

Figure 7.15: The comparison of T/T_c on a/a_c for finite superlattice system $j = 10$ in various b/a_c with the single layer. (a) $b/a_c = 0.01$, (b) $b/a_c = 0.1$, (c) $b/a_c = 1$, (d) single layer

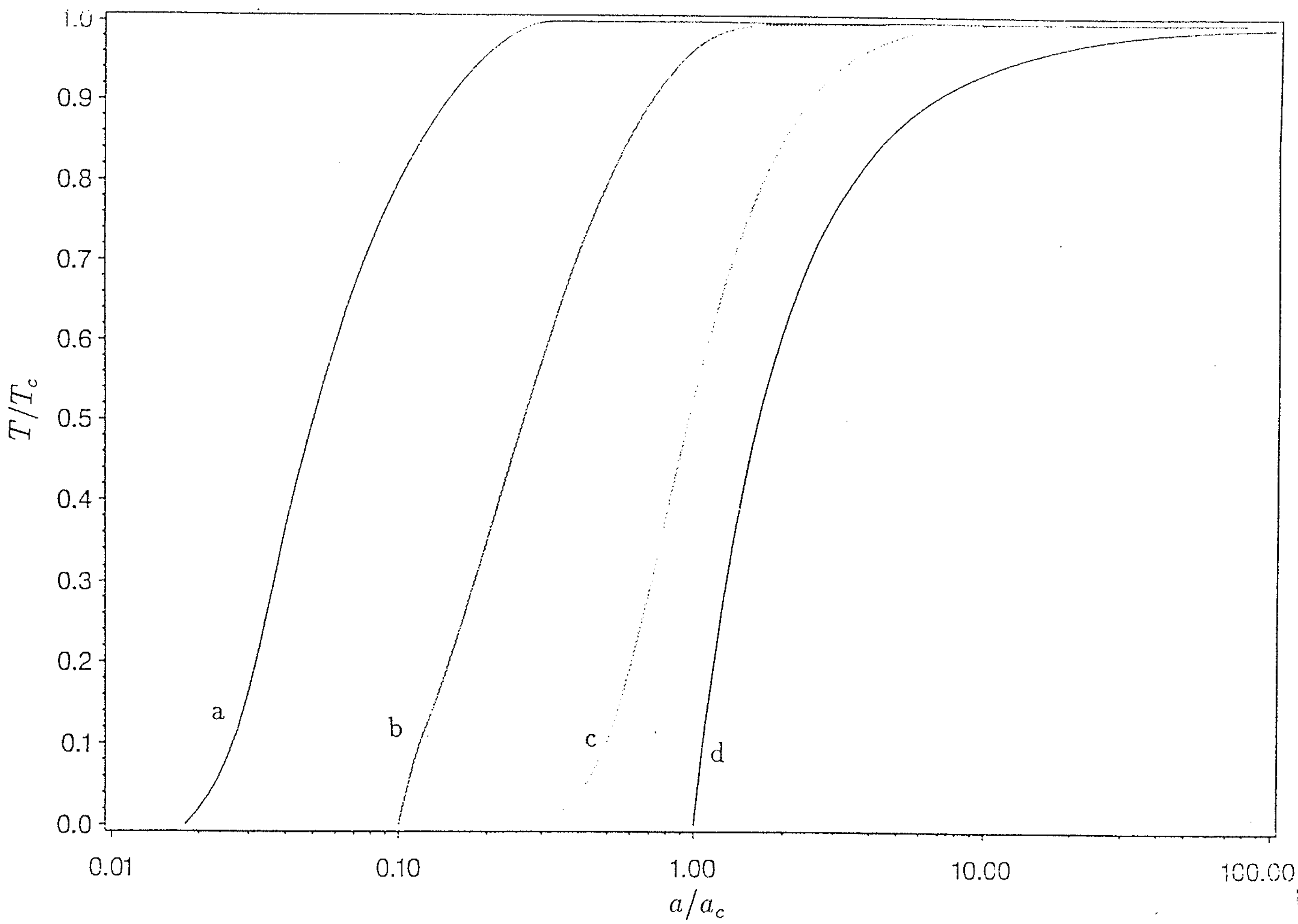

Figure 7.16: The comparison of T/T_c on a/a_c for a infinite superlattice system and the single layer. (a) $b/a_c = 0.01$, (b) $b/a_c = 0.1$, (c) $b/a_c = 1.0$, (d) single layer.

Appendix A

Sine and Cosine Integrals

In this appendix we present the definition of the Sine and Cosine integrals arising in the method, together with approximation of the functions in various limits.

These integrals are denoted by $Si(x)$, and $Ci(x)$, and defined as

$$Ci(x) = -\int_x^\infty \frac{\cos t}{t} dt = \gamma_e + \ln x + \int_0^x \frac{\cos t - 1}{t} dt \tag{0.1}$$

and

$$Si(x) = -\int_x^\infty \frac{\sin t}{t} dt = -\frac{\pi}{2} + \int_0^x \frac{\sin t}{t} dt, \tag{0.2}$$

where $\gamma_e = 0.5772156649$ is Euler's constant.

The Cosine integral is an even function and the Sine integral is odd. Close to $x = 0$, the functions can be approximated by

$$Si(x) \approx x \exp(-\frac{x^2}{18}) \qquad |\, x \,| \leq 2.2 \tag{0.3}$$

and

$$Ci(x) \approx \frac{x^2}{4} \exp(-\frac{x^2}{14}) \qquad |\, x \,| \leq 2.5. \tag{0.4}$$

For large x the approximations are

$$Si(x) \approx \frac{\pi}{2} - \frac{x \cos(x)}{x^2 + 2} - \frac{\sin(x)}{x^2 + 6} \tag{0.5}$$

and

$$Ci(x) \approx \frac{x \sin(x)}{x^2 + 2} - \frac{\cos(x)}{x^2 + 6}. \tag{0.6}$$

Appendix B

An Integration

In this appendix, we evaluate the expression

$$\begin{aligned} K(x) &= \frac{a}{\tau}\int_0^\infty [\frac{\sin(ax)}{ax} - \cos(ax) - 2Ci(ax) - (ax)Si(ax)]\cosh^{-2}(\frac{x}{\tau})dx \\ &= \frac{a}{\tau}\int_0^\infty dxJ(ax)\cosh^{-2}(\frac{x}{\tau}), \end{aligned} \tag{0.2}$$

which appears in Chapter 7, Section (2.2). We first consider a general expression with parameter a.

(1). We have

$$I_1 = \frac{a}{\tau}\int_0^\infty dx\cos(ax)\cosh^{-2}(\frac{x}{\tau}).$$

Let $\frac{x}{\tau} = v$, $dx = \tau dv$, and we find[41]

$$I_1 = \frac{a^2\tau\pi}{2}\sinh^{-1}(\frac{a\tau\pi}{2}). \tag{0.3}$$

(2). We next consider

$$\begin{aligned} I_2 &= \frac{a}{\tau}\int_0^\infty dxCi(ax)\cosh^{-2}(\frac{x}{\tau}) \\ &= -\frac{a}{\tau}\int_0^\infty dx\cosh^{-2}(\frac{x}{\tau})\int_{ax}^\infty \frac{dz}{z}\cos z. \end{aligned} \tag{0.5}$$

Let $y = z/ax$, for which $dz = (ax)dy$, and we find

$$\begin{aligned} I_2 &= -\frac{a}{\tau}\int_0^\infty dx\cosh^{-2}(\frac{x}{\tau})\int_1^\infty \frac{dy}{y}\cos(axy) \\ &= -\frac{a}{\tau}\int_1^\infty \frac{dy}{y}\int_0^\infty dx\frac{\cos(axy)}{\cosh^2(x/\tau)} \\ &= -\frac{a}{\tau}\int_1^\infty \frac{dy}{ay^2}\int_0^\infty du\frac{\cos(u)}{\cosh^2(u/a\tau y)} \\ &= -\frac{1}{\tau}\int_1^\infty \frac{dy}{y^2}\int_0^\infty du\frac{\cos(u)}{\cosh^2(u/a\tau y)}, \end{aligned} \tag{0.7}$$

where $u = axy$ and $dx = du/ay$. Since

$$\int_0^\infty du\frac{\cos(u)}{\cosh^2(u/ay\tau)} = \frac{\pi(ay\tau)^2}{2}\sinh^{-1}(\frac{ay\tau\pi}{2}),$$

we have

$$I_2 = -\frac{\pi a^2\tau}{2}\int_1^\infty dy\sinh^{-1}(\frac{ay\tau\pi}{2}).$$

Letting $g = ay\tau\pi/2$, for which $dy = dg[2/(a\tau\pi)]$, we find

$$\begin{aligned} I_2 &= -a\int_{a\tau\pi/2}^\infty dg\sinh^{-1}g \\ &= a\ln[\tanh(\frac{a\tau\pi}{4})]. \end{aligned} \tag{0.9}$$

(3). We next have

$$\begin{aligned} I_3 &= \frac{a}{\tau}\int_0^\infty \frac{\sin(ax)}{ax}\cosh^{-2}(\frac{x}{\tau}) \\ &= \frac{1}{\tau}\int_0^\infty \frac{\sin(ax)}{x}\cosh^{-2}(\frac{x}{\tau}). \end{aligned} \tag{0.11}$$

Since

$$\begin{aligned} \frac{dI_3}{da} &= \frac{1}{\tau}\int_0^\infty dx\cos(ax)\cosh^{-2}(\frac{x}{\tau}) \\ &= \frac{a\pi\tau}{2}\sinh^{-1}(a\pi\tau/2), \end{aligned} \tag{0.13}$$

we find

$$I_3 = \int_0^a \frac{dI_3}{da} dx = \frac{\pi\tau}{2} \int_0^a x dx \sinh^{-1}(x\pi\tau/2).$$

Letting

$$u = x \quad dx = du,$$

for which

$$dv = dx \sinh^{-1}(x\pi\tau/2) \quad v = \frac{2}{\pi\tau} \ln[= \tanh(x\pi\tau/4)],$$

we obtain

$$\begin{aligned} I_3 &= \frac{\pi\tau}{2} \int_0^a x dx \sinh^{-1}(x\pi\tau/2) \\ &= a \ln[\tanh(a\pi\tau/4) - \int_0^a dx \ln[\tanh(x\pi\tau/4)]. \end{aligned} \quad (0.15)$$

(4). We finally consider

$$\begin{aligned} I_4 &= \frac{a}{\tau} \int_0^\infty dx(ax) Si(ax)] \cosh^{-2}(\frac{x}{\tau}) dx \\ &= -\frac{a^2}{\tau} \int_0^\infty dx x \cosh^{-2}(\frac{x}{\tau}) \int_1^\infty \frac{dz}{z} \sin(axz) \\ &= -\frac{a^2}{\tau} \int_1^\infty \frac{dz}{z^3} \int_0^\infty x dx \sin(ax) \cosh^{-2}(\frac{x}{z\tau}) \\ &= \frac{a^2}{\tau} \int_1^\infty \frac{dz}{z^3} [\frac{d}{da} \int_0^\infty dx \cos(ax) \cosh^{-2}(\frac{x}{z\tau})] \\ &= \frac{a^2}{\tau} \int_1^\infty \frac{dz}{z^3} \frac{d}{da} [\frac{a\pi}{2(1/\tau)^2 \sinh(a\pi\tau z/2)(1/z^2)}] \\ &= \frac{a^2\tau\pi}{2} \int_1^\infty \frac{dz}{z} \frac{d}{da} [\frac{a}{\sinh(a\pi\tau z/2)}] \\ &= \frac{a^2\tau\pi}{2} \int_1^\infty \frac{dz}{z} [\frac{1}{\sinh(a\pi\tau z/2)} - (\frac{a\pi\tau z}{2}) \frac{\cosh(a\pi\tau z/2)}{\sinh^2(a\pi\tau a/2)}] \\ &= \frac{a^2\tau\pi}{2} [\int_1^\infty \frac{dz}{z \sinh(a\pi\tau z/2)} - \frac{1}{\sinh(a\pi\tau/2)}]. \end{aligned} \quad (0.17)$$

Since

$$\int_1^\infty \frac{dz}{z \sinh(bz)} = -(1/b) \ln[\tanh(b/2)] + (1/b) \int_1^\infty \frac{dz}{z^2} \ln[\tanh(bz/2)],$$

we obtain

$$
\begin{aligned}
I_4 &= \frac{a^2\tau\pi}{2}\{-\frac{2}{a\pi\tau}\ln[\tanh(a\pi\tau/4)] \\
&+ \frac{2}{a\pi\tau}\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)] - \frac{1}{\sinh(a\pi\tau/2)}\} \\
&= -a\ln[\tanh(a\pi\tau/4)] + a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(a\pi\tau z/4)] \\
&- \frac{a^2\tau\pi}{2\sinh(a\pi\tau/2)}. \qquad (0.19)
\end{aligned}
$$

Thus, summing the various terms, we have

$$
\begin{aligned}
K(x) &= \frac{a}{\tau}\int_0^\infty dxJ(ax)\cosh^{-2}(\frac{x}{\tau}) = -I_1 - 2I_2 + I_3 - I_4 \\
&= -\int_0^a dx\ln[\tanh(x\pi\tau/4)] - a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)] \\
&= -\{\int_0^\infty dx\ln[\tanh(x\pi\tau/4)] - \int_a^\infty dx\ln[\tanh(x\pi\tau/4)] \\
&+ a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)]\}. \qquad (0.21)
\end{aligned}
$$

Since

$$
\begin{aligned}
\int_0^\infty dx\ln[\tanh(x\pi\tau/4)] &= \frac{4}{\pi\tau}\int_0^\infty dt\ln\frac{1-\exp(-2t)}{1+\exp(-2t)} \\
&= -\frac{\pi}{2\tau}, \qquad (0.22)
\end{aligned}
$$

where $t = \pi\tau x/4$, we obtain

$$
\begin{aligned}
K(x) &= \frac{a}{\tau}\int_0^\infty dxJ(ax)\cosh^{-2}(\frac{x}{\tau}) \\
&= -\{-\frac{\pi}{2\tau} - \int_a^\infty dx\ln[\tanh(x\pi\tau/4)] + a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)]\} \\
&= \frac{\pi}{2\tau} + \int_a^\infty dx\ln[\tanh(x\pi\tau/4)] - a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)]\}, (0.23)
\end{aligned}
$$

or, letting

$$x = az \qquad dx = adz; \qquad ,$$

$$x \longrightarrow \infty \qquad z \longrightarrow \infty \quad ,$$

and

$$x = a \qquad z = 1 \qquad ,$$

we have

$$\int_a^\infty dx \ln[\tanh(x\pi\tau/4)] = \int_1^\infty adz \ln[\tanh(\pi\tau az/4)].$$

We finally obtain

$$\begin{aligned} K(x) &= \frac{a}{\tau}\int_0^\infty dx J(ax)\cosh^{-2}(\frac{x}{\tau}) \\ &= \frac{\pi}{2\tau} + a\int_1^\infty dz \ln[\tanh(za\pi\tau/4)] - a\int_1^\infty \frac{dz}{z^2}\ln[\tanh(az\pi\tau/4)] \\ &= \frac{\pi}{2\tau} + a\int_1^\infty dz(1-\frac{1}{z^2})\ln[\tanh(za\pi\tau/4)]. \end{aligned} \tag{0.25}$$

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