APPLICATIONS OF A LINEAR RESPONSE FORMALISM TO THE KONDO SYSTEM

Mesbahuddin Ahmed

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University of Kent at Canterbury

England

CONTENTS

CHAPTER PAGE

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ABSTRACT

The electrical conductivity of a metallic system containing a very low concentration of paramagnetic impurities (commonly known as a Kondo system) is investigated by applying the linear response formalism. Starting from the s-d exchange Hamiltonian, the Nagaoka equations are re-formulated in the presence of a uniform electromagnetic field and a finite concentration of impurities. These self-consistent, closed set of equations are solved diagrammatically and it is shown that for s-wave scattering only, or more generally if only a single phase shift of the exchange interaction is non zero, the vertex corrections drop out. The calculations of conductivities at high and low temperatures, compared to the Kondo temperature, T_K, where the perturbation theory breaks down, within the response formalism then give the same results as those of Nagaoka. Our investigation also substantiates the approximation that the Kondo system relaxes with a characteristic time, τ , provided the concentration of impurities is so low that the interaction between the impurities can be neglected.

The same formalism has been used to calculate analytically the frequency-dependent conductivity at low temperatures. Because of the approximations involved in the calculations, our result is valid for frequencies very much less than 10^{12}Hz. The real and imaginary parts of the complex conductivity are written down in terms of a dimensionaless parameter in the 'pure' and 'dirty' limits (concentration of impurities, $c \sim 10^{-5}$ or more). In contrast with the numerical calculations of Murata and Wilkins, the

real part of the conductivity does not show a peak with respect to the frequency. In the 'pure' limit, the conductivities can be expressed as a universal function of impurity-concentration, and in the 'dirty' limit they are independent of it. These results are in agreement with the calculations of Murata and Wilkins. The predicted peak has not yet been observed experimentally.

The basic equations are derived again, taking an extended exchange interaction, with finite concentration of impurities but this time in the absence of the electric field. By following the same procedure, these equations have been solved for s and p wave scattering together. The vertex function for high temperatures has been evaluated from an integral equation formed through the Ward's identity. The electrical conductivity at high temperatures is calculated and a third order term in the exchange interaction is found in the coefficient of the leading logarithmic term as a correction. This term occurs due to the interference of s and p wave scattering and it has been shown that for a particular ratio of the strengths of s and p wave scattering, the leading logarithmic term can vanish giving an entirely new high temperature behaviour. The next highest order term has been calculated, and it is shown that this term does not vanish for the particular ratio when the leading term vanishes. Some experimental results are discussed in the light of the present theory. The approximate expression for the conductivity at low temperatures has been found. At absolute zero temperature, the effect of inclusion of p wave scattering is a significant reduction in the conductivity.

For weak p-wave scattering, the conductivity at low temperatures is found to depend on p-wave scattering only.

CHAPTER 1 INTRODUCTORY REMARKS ON THE KONDO PROBLEM

1.1 Early Experimental Work

The study of dilute alloys of transition metal and rare-earth ions in non-magnetic hosts has a long history. In 1930, Meissner and Voigt[1] observed that the electrical resistivity of certain metals, particularly of 'pure' gold, decreased first and then gradually increased, by a few per cent, as temperature is decreased to below 10°K. This was studied more closely by De Haas, De Boer and Van den Berg[2] and they found a minimum in the resistance-temperature curve of 'pure' gold (impurity $<10^{-4}$%). Linde[3] carried out a series of investigations on the specific increase in the resistivity when small amounts of normal and transition metals were added to the noble metals, (Cu, Ag and Au). He observed that Linde's rule[4] is valid for the addition of normal metals but not for transition metals. Later, Gerritsen and Linde's[5] experiments on electrical resistivity of Ag-Mn alloys showed a minimum for a concentration of about 0·1 at % Mn in Ag. Since then, the same phenomenon has been observed in many other alloys.[6-21]

For many years the subject remained obscure despite experimental studies, and in the absence of proper theoretical explanation the anomalous behaviour remained a mystery. It is only in recent years that an understanding of the nature of the problem has been attained. Gradually, a number of phenomena became quite well established. Anomalies in the thermodynamic and transport properties of the alloys were correlated with the existence of a local

moment on the impurity ions[22], as indicated by high temperature susceptibility measurements[23,24]. The principal effects observed were the following:

(1) A resistance minimum occurred at low temperature. This was remarkably different behaviour from that found in 'normal' alloys where the low temperature resistivity became a temperature independent function dominated by defect and ordinary impurity scattering. Such anomalous effects were observed, for example, in numerous gold-, silver- and copper-based transition metal alloys[6-21]. In Cu-Fe the temperature of the minimum, T_{min} was found to vary with the impurity concentration c as $T_{min} \propto c^{1/5}$[15].

(2) The high temperature magnetic susceptibility χ, approximately obeyed a Curie-Weiss law, $\chi(T) = \frac{C}{(T+\theta)}$ where θ was generally of the same order as T_{min}[22] and C is a constant. For small impurity concentration, $\chi(T)$ was proportional to concentration and no antiferromagnetic order was observed. But deviations from the Curie and Curie-Weiss law were observed at low temperatures[25,26].

(3) The magnetoresistance was found negative at temperatures below T_{min}[7,27].

(4) The specific heat exhibited a peak at 6°K in Cu-Fe alloys[28,29]. The associated entropy under the specific heat curve was consistent with the loss of spin degree of freedom as the temperature dropped toward zero. A similar peak was suggested in Cu-Cr[29,30] specific heat data with entropy R ℓn 2.5 per mole of

impurity (R is the gas constant per mole).

(5) Very large and negative thermoelectric power was found in the same temperature region where the specific heat and resistivity were anomalous[31,32].

Similarly, anomalies were observed in the linewidth of NMR[33-35] and Mössbauer spectra[36,37].

No theory proposed before 1964 satisfactorily explained the available experimental results. Attempts to explain experimental data followed in two different directions. The first concerned the conditions for the existence and stability of localized moments in the system. The second studied the effects of localized moments on the properties of the host metal. Both of these have been studied extensively on the basis of different models.

1.2 The Kondo Problem

The study of the existence of localized moments in metals started with the work of Friedel[38]. By introducing the concept of a 'virtual bound state' he explained why local moments are more stable in monovalent metals than in polyvalent metals. Anderson and Wolff[39,40] proposed simple models to establish criteria for the existence of localized moments. Long before that, Zener[41] proposed a model of ferromagnetic transition metals where an exchange interaction between the localized d electrons and itinerant s electrons is assumed to be the cause of ferromagnetism of the 3d metals. This model has also been applied to magnetic alloys where an impurity spin of fixed magnitude is thought to interact with the spins of the conduction electrons (the s-d exchange model). Schrieffer and Wolff[42] showed that this type of interaction can be obtained from the Anderson model if the

width of the spin split of d levels is small compared to the distance of these levels from the Fermi surface.

For a long time, it was believed that the ordinary perturbation theory could account for the anomalous properties of dilute alloys. Yosida[43] calculated the resistivity due to spin disorder scattering to the first Born Approximation and found that the temperature dependence of the relaxation time τ was too small to account for the rise in the resistivity at low temperatures. Kondo realized that as the resistance-minimum was a widely observed phenomenon, it should be possible to explain it using a very simple model. He carried the calculation one step further, to the second Born Approximation[44]. In the second Born Approximation, intermediate states come into the picture. The amplitudes of two probable processes of spin flip scattering (say $K\uparrow \rightarrow K'\downarrow$) do not cancel, because the probability of these two processes occurring are not the same. When integrated over the intermediate energy, it leads to a term containing $\ell n\ T$. The expression for resistivity, R(T) due to the exchange scattering was found to be

$$R(T) = c\ R_m[1 + J\ N(0)\ \ell n\ T/D] \qquad (1.1)$$

where c is the concentration of impurities, N(0) is the density of band states per atom near the Fermi surface, D is the cut off parameter of the order of band width and R_m is the resisitivity calculated in the first Born Approximation (we choose units such that $\hbar = K_\beta = 1$). The logarithmic term increases as the temperature decreases if the strength of exchange interaction, J is negative. This term added to normal phonon scattering gave remarkable

agreement with experimental data showing resistance-minimum. Kondo concluded that J should be negative for alloys showing resistance-minimum. Furthermore, when lattice scattering ($R_L(T) \propto T^5$) is added to Eq.(1.1), the total resistivity may be shown to have a minimum at $T_{min} \propto c^{1/5}$.

The logarithmic term can be viewed as arising out of the 'internal structure' of the localized spin from which the conduction electrons scatter. There are two degenerate internal states, spin up and spin down. Since the result of any particular scattering is dependent upon the spin orientation, it is also dependent upon the previous scattering. Mathematically, it is a consequence of the non-commutability of the spin operators, $S_+S_- - S_-S_+ \neq 0$. The Fermi factors which occur in the intermediate states of a perturbation calculation no longer cancel as happens for normal potential scattering. In the third order, they add, and the summation over intermediate momenta generate the logarithmic dependence of the scattering lifetime near the Fermi surface.

Kondo's calculation[44], while explaining some features of the resistivity data, brought in new difficulties. Eq. (1.1) implies that the resistivity diverges as $T \to 0$. This cannot be the case, since all scattering is limited by unitarity. It must be noted that Eq. (1.1) represents only the first two terms of the expansion. The second term dominates over the first as $T \to 0$, however small $J\,N(0)$ may be. It was found that in higher order similar logarithmic terms were present and these could be summed as a geometric series, giving

$$R(T) = c\,R_m[1 - J\,N(0)\,\ln T/D]^{-1} \qquad (1.2)$$

which has a pole for negative (antiferromagnetic) sign of J at the 'Kondo temperature, T_K given by

$$T_K = D\, e^{-1/|J|N(0)} \qquad (1.3)$$

This signifies the breakdown of perturbation theory. Such behaviour usually signals an instability of the normal Fermi sea, as was earlier recognized in the theory of superconductivity[45]. In that case a phase transition takes place which brings in a new 'superfluid' state. Because of the limited number of spin degrees of freedom, the Kondo system behaves in many ways like a zero dimensional system, and hence a usual phase transition does not take place. Experimentally also the thermodynamic properties pass smoothly from their high to low temperature values.

1.3 Theoretical Development

A large number of attempts have been made to explain the low temperature behaviour of the Kondo system. They may be classified into three groups[46]; (1) analytic continuations of the dominant terms in high temperature perturbation theory to low temperatures, $T < T_K$[47-52], (2) variational techniques at $T = 0$[55-57] to determine ground state properties and the low lying excitation spectrum and (3) the concept of 'localized spin fluctuation'[58-60] which starts from non-magnetic states and allows gradual transition to the magnetic states. We shall restrict our treatment to (1).

The most widely used theories of the first type are those of Abrikosov[47], Suhl[48] and Nagaoka[49] as extended by Hamann[50], Bloomfield[51], Zittartz and Müller-Hartmann[52]. Abrikosov[47] replaced the local spin by a pseudo-fermion

and summed up the special 'parquet' diagrams to calculate the perturbation series. Suhl[48] formulated the problem in terms of dispersion theory while Nagaoka[49] wrote Green's function equations-of-motion which were then truncated and solved. Later theories were shown to be equivalent[53], although their identity was not apparent from the outset. It is the approach of Nagaoka[49,54] which we intend to follow later.

Using the retarded double time Green's function, Nagaoka[49] derived a closed set of equations for two single electron Green's functions. This was reduced to a nonlinear singular integral equation for the non-spin flip part of the T-matrix by Hamann[50]. From his solution the temperature dependence of the resistivity was calculated and found to be in qualitative agreement with experiment above T_K. As $T \to 0$, R(T) approached the unitarity limit. The specific heat was initially found to be zero, but this discrepancy with experiment was resolved through an essentially exact solution for T-matrix later carried out by Bloomfield and Hamann[51]. A pronounced maximum in the specific heat, $C_V(T)$ was found at $T \sim \frac{1}{3}T_K$. Zittartz and Müller-Hartmann[52] then showed from the exact solution that $C_V(T) \propto \ell n^{-4} T/T_K$ as $T \to 0$.

The susceptibility has been a slightly more difficult problem since it cannot be directly calculated from the T-matrix. A theory due to Zittartz[61], based upon essentially the same physical assumptions as the truncation by Nagaoka, has shown that $\chi(T)$ becomes negative at low temperatures. Though such a result is inconsistent, it does indicate the tendency of conduction electrons to compensate

the local spin for $T < T_K$. Later, Bloomfield, Hecht and Sievert[62] have extended the Nagaoka theory to finite magnetic fields and found a similar negative susceptibility at low temperatures in the presence of small magnetic fields.

The earliest of the variational theories was developed by Yosida[55]. Other later attempts[56,57] predicted a ferromagnetic instability for $J > 0$ in disagreement with perturbation expansions . For antiferromagnetic coupling, $J<0$, all variational theories assume a singlet ground state. Mattis'[63] proof, and other results from finite temperature theories[64], support this assumption. Yosida[55] started with a trial wave function in which one electron above the Fermi sea was paired in a singlet way with the local moment. Then the coupling parameter was varied to minimize the ground state energy. In higher orders successive numbers of particle-hole pairs were added to the single electron. As increasing numbers of pairs accumulated, it was shown that the net binding energy grew, and approached T_K in the limit. Thus, the formation of the singlet bound state led to small decrease in energy.

The third line of investigation started with the work of Lederer and Mills[58], Rivier[59] and Suhl[60]. The idea of this approach was to begin with Anderson model[65] and to use many-body perturbation theory starting with the assumption that the ground state is a non-magnetic one. This is called the 'localized spin fluctuation' theory. Now, in cases in which the impurity is indeed not very magnetic, for example Mn in Al[66], this theory is very successful. One obtains a non-singular slowly decreasing susceptibility, and a resistivity which may increase or

decrease as T^2. Again, since the localized state is indeed non-magnetic, such a theory works with renormalised parameters over any limited temperature range. Hamann and Schrieffer[96] showed how this renormalisation works in such a way as to give Kondo temperature, and also worked out the relationship between high and low temperature regimes.

Thus the qualitative features of the Kondo anomalies appear to be reasonably explained. Below T_K all theories predict a very strong coupling of the conduction electron spin and the impurity moment. At T = 0, the coupling is so strong that the spin nonflip scattering at the Fermi surface reaches the unitarity limit, and a singlet ground state is formed. This state has a binding energy of order T_K and its formation is accompanied by a specific heat anomaly. The entropy under the specific heat curve is of order $\ell n\ 2$[62,67], corresponding to the loss of the local spin degree of freedom. Negative magnetoresistance is understood as the tendency of a magnetic field to break up the singlet pairing, and hence to reduce the scattering cross section.

1.4 Comparison of Theory and Experiment

At high temperatures, $T > T_K$, all physical properties can be calculated by applying perturbation theory and the results are in good agreement with experimental data. However, several discrepancies still exist between theory and experiment. One which is clearly apparent is that the width of the transition from high to low temperature behaviour is predicted to be too broad. For example, the width of the specific heat anomaly is theoretically about two decades temperature[62], while experiment indicates only one decade[68]. The resistance anomaly is similarly predicted to be considerably broader than the $1\frac{1}{2}$ decades found

experimentally[69].

A number of more serious quantitative disagreements with experiment occur at low temperatures, $T << T_K$. By taking care to eliminate the effects of interactions between impurities, it has been found that simple power law in T governs the low temperature behaviour of the Kondo system[70-72]. At low temperatures, it was observed that the resistivity varied as

$$R(T) = R(0)(1 - a\,T^2) \text{ for } \underline{Pd}Cr^{(71)}$$

and for $\underline{Cu}Fe^{(72)}$ (with Fe concentration, $c = \cdot 6 \times 10^{-4}$) and also

$$R(T) = R(0)[1 - a(T\,\ell n\,T/b)^2] \text{ for } \underline{Au}V,\ \underline{Cu}Cr^{(73)}$$

and also for $\underline{Cu}Fe^{(73)}$ (with $c = \cdot 13 \times 10^{-4}$ to $\cdot 4 \times 10^{-3}$). But the theory predicts an infinite slope of the resistivity at T = 0 as a function of T(zero slope for R as a function of $\ell n\ T/T_K$) and for very low temperature a negative curvature of R(T) for $s \geq \frac{1}{2}$. However, other predictions of the theory at high temperatures seem to be in good agreement with the experimental data.

A quite different behaviour has been observed in alloys such as $\underline{Rh}Fe$, $\underline{Ir}Fe$, $\underline{Pd}Co^{(74-76)}$ etc. where the impurity contribution to resistivity increases with increasing temperature and decreases strongly with decreasing temperature. This has been discussed in terms of positive J[44]. But the susceptibility measurements show a very substantial decrease in the magnetic moment at low temperatures[77]. They also show a specific heat anomaly at low temperatures[78] and there are Mössbauer anomalies similar to that in $\underline{Cu}Fe^{(79)}$. Thus, except for resistivity, these results indicate that they are negative J systems.

Attempts have been made on the basis of 'localized spin fluctuation'[80] model and two-band model[81] to explain the resistivity of these alloys. But, these systems are not well understood yet.

Our object has been to study the nature of the exchange scattering and to try to explain the experimental data with the existing theory. In the second chapter we develop Nagaoka equations with finite concentration of magnetic impurities in the presence of a uniform electromagnetic field, $\underset{\sim}{A}(t)$. We solve these equations (Chapter 3) for $\underset{\sim}{A}(t) = 0$ and $A(t) \neq 0$. There we show explicitly that for constant J, the 'vertex corrections'[82] drop out when we average over the impurity positions. We then recover Nagaoka's result for the conductivities at high and low temperatures. As a by-product of applying the linear response formalism to the Kondo system, we have succeeded in calculating analytically the frequency dependent conductivity at low temperatures (Chapter 4). In Chapter 5, we reformulate the equations with finite concentration of magnetic impurities - this time with extended exchange interaction, and present a formal solution. In Chapter 6, we solve the equations for s and p wave scattering only. We calculate the resistivities at high and low temperatures and present some discussion on the results. In the final chapter we discuss some aspects of the Kondo system and attempt to indicate the nature of future work within our formulation.

CHAPTER 2 FORMULATION OF THE EQUATIONS

2.1 Introduction

The explanation of the resistance minimum given by Kondo in his celebrated paper[44] turned out to be extremely stimulating. Kondo pointed out that the resistance minimum arose as a many-body effect from the spin dependent scattering of conduction electrons from the localized moments. This can be viewed as follows: the scattering of an electron by the impurity depends on the fact that a previous such event had taken place, and hence an indirect electron-electron interaction is generated. This is schematically shown in the diagram (Fig. 1). A similar case was found previously in the

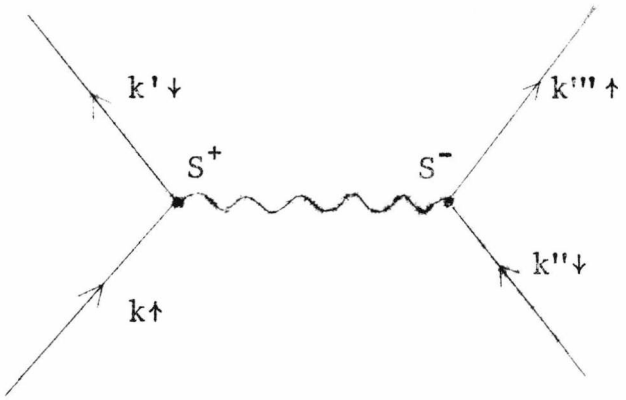


Figure 1. Schematic diagram of the indirect electron-electron interaction in the Kondo effect.

two-particle t-matrix for scattering through the indirect (via phonons) electron-electron interaction which leads to superconductivity. After Kondo's paper, a large number of nonperturbative attempts have been made to describe the state of the system for temperatures $T < T_K$. We shall restrict ourselves to the equation-of-motion method due to Nagaoka[49,54] and consider the case when potential scattering is absent. Some parts of the derivation overlap with

that of Nagaoka, we shall, nevertheless, include them for the sake of completeness.

2.2 The Hamiltonian

We take the s-d exchange Hamiltonian which starts from the assumption that a localized magnetic moment exists at the impurity site. Friedel[28] and Wolff[40] have worked out how such a moment could exist in a metallic environment and Anderson[39] showed why some transition metal impurities in noble metal would show magnetic behaviour and others would not. In the s-d exchange Hamiltonian the impurity spin of fixed magnitude is coupled with the spins of the conduction electrons through an exchange interaction. For N_i impurities distributed randomly throughout the system such that the impurity concentration, $c = N_i/N$ (where N is the number of atoms in the crystal) is very low to enable us to neglect the interaction between the impurities, we take the model Hamiltonian for the Kondo system given by,

$$H = H_o + \sum_{\alpha} H_{ex}^{\alpha} \tag{2.1}$$

where

$$H_o = \sum_{k\sigma} \varepsilon_k C_{k\sigma}^{+} C_{k\sigma} \tag{2.2}$$

and

$$H_{ex}^{\alpha} = -\frac{J}{2N} \sum_{kk'} e^{i(\underline{k}'-\underline{k})\cdot\underline{R}\alpha} [(C_{k\uparrow}^{+} C_{k'\uparrow} - C_{k\downarrow}^{+} C_{k'\downarrow}) S_z^{\alpha}$$

$$+ C_{k\uparrow}^{+} C_{k'\downarrow} S_{-}^{\alpha} + C_{k\downarrow}^{+} C_{k'\uparrow} S_{+}^{\alpha}] \tag{2.3}$$

Equation (2.2) is the conduction electron kinetic energy; Eq.(2.3) represents the s-d interaction. Here $C_{k\sigma}^{+}$ and $C_{k\sigma}$ are the creation and annihilation operators of the conduction electron with wave vector $\underline{k}$ and spin σ , ε_k being its energy

measured from the Fermi surface. We take J which represents the strength of the exchange coupling between the conduction electrons and the local spin $\underset{\sim}{S}^{\alpha}$, to be constant. The positive and negative signs of J indicate ferromagnetic and antiferromagnetic coupling respectively. Later on we shall consider the effect of the extended exchange interaction. The localized orbital is assumed to be occupied by just one electron - this assumption is inherent in the Hamiltonian. Also $S^{\alpha}_{\pm}$, S^{α}_{z} are the components of the spin operator $\underset{\sim}{S}^{\alpha}$. For simplicity, we shall restrict our treatment to the case of $S^{\alpha} = \frac{1}{2}$ only.

Let us now introduce, the single particle time dependent Green's function[83] defined by

$$G_{kk'}(t,t') = -i< TC_{k'\uparrow}(t)C^{+}_{k\uparrow}(t') > \qquad (2.4)$$

Here <....> denotes the averaging over the grand canonical ensemble, i.e. the expectation value of an operator, χ is given by

$$< \chi > = \frac{Tr[e^{-\beta H}\chi]}{Tr[e^{-\beta H}]} \qquad (2.5)$$

where Tr denotes the trace and $\beta = 1/T$. [For convenience, we shall use units such that, Planck's constant divided by 2π and Boltzmann constant are equal to unity, i.e. $\hbar = k_{\beta} = 1$]. $C_k(t)$, $C^{+}_k(t)$ are Heisenberg operators in which times evolve as

$$C_k(t) = e^{iHt}C_k e^{-iHt} \qquad (2.6)$$

and T orders the imaginary parts of t,t'. The boundary condition is

$$G_{kk'}(t,t')\Big|_{t=o} = - G_{kk'}(t,t')\Big|_{t= -i\beta} \qquad (2.7)$$

(the minus sign appears because we are dealing with Fermions) which states that the Green's function is analytic for the complex values of the time arguments in the period 0 to $-i\beta$. The Fourier expansion of it is given by

$$G_{kk'}(\omega_n,t') = \frac{1}{-i\beta}\int_o^{-i\beta} G_{kk'}(t,t')e^{-\omega_n t}dt \qquad (2.8)$$

where, $\omega_n = (2n + 1)\pi/\beta$, $n = 0, \pm1, \pm2,\ldots$, the odd Matsubara frequency[82] for Fermions.

2.3 The Equations of Motion

We now develop the equation of motion for the Green's function in the presence of a uniform electromagnetic field, $\underset{\sim}{E}(t) = -\frac{\partial \underset{\sim}{A}(t)}{\partial t}$. Using

$$i\frac{dC_k(t)}{dt} = [C_k,H]_- \qquad (2.9)$$

the equation of motion of the Green's function $G_{kk'}(t,t')$ can be written as

$$i\frac{dG_{kk'}(t,t')}{dt} = \delta(t-t')\delta_{kk'} + \varepsilon_{k'}(t)G_{kk'}(t,t') - \frac{J}{2N}\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha}\,\Gamma^{\alpha}_{k\ell}(t,t') \qquad (2.10)$$

Here the Green's function depends explicitly on t and t' and not just on (t-t') as is usually the case in the absence of the field. We also defined

$$\Gamma^{\alpha}_{kk'}(t,t') = -i\langle T[C_{k'\uparrow}(t)S^{\alpha}_z(t) + C_{k'\downarrow}(t)S^{\alpha}_-(t)]C^{+}_{k\uparrow}(t')\rangle \qquad (2.11)$$

It can be easily verified that the Green's function $\Gamma^{\alpha}_{kk'}$, also satisfies the same boundary condition (2.7) and hence has the same Fourier expansion. Since, the first order terms in the field $\underset{\sim}{A}(t)$ is enough to calculate transport properties of the system, we shall neglect higher order terms in the field, i.e. we can take

$$\varepsilon_k(t) \cong \varepsilon_k - a_o(\underset{\sim}{A}_{\omega}.\underline{k})e^{-i\omega t} \tag{2.12}$$

where $a_o = e/m^*$, e is the charge and m* is the effective mass of the electron and the response to the field is taken to be of the form $\underset{\sim}{A}(t) = \underset{\sim}{A}_{\omega}\, e^{-i\omega t}$ where ω is the frequency of the field. Then using the Fourier transforms of $G_{kk'}$ and $\Gamma^{\alpha}_{kk'}$, Eq. (2.10) can be written as

$$\begin{aligned}\sum_{\omega_n} i\omega_n G_{kk'}(\omega_n,t')e^{\omega_n t} &= \delta_{kk'}\delta(t-t') \\ &+ \varepsilon_{k'}\sum_{\omega_n} G_{kk'}(\omega_n,t')e^{\omega_n t} \\ &- a_o(\underline{A}\omega.\underline{k}')\sum_{\omega_n} G_{kk'}(\omega_n,t')e^{(\omega_n - i\omega)t} \\ &- \frac{J}{2N}\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\sum_{\omega_n}\Gamma^{\alpha}_{k\ell}(\omega_n,t')e^{\omega_n t}\end{aligned} \tag{2.13}$$

For convenience we set, $\omega = i\omega_p$, $\omega_p = 2\pi p/\beta$, $p = 0, \pm1, \pm2\ldots$, and evaluate the response at points ω_p and later we make analytic continuation in the upper half plane, according to $i\omega_p \to \omega + i0+$ (0+ is a positive infinitestimal) to extend the results for all frequencies. Multiplying both sides of (2.13) by $e^{-\omega_n' t}$ and integrating over t from 0 to $-i\beta$, we get

$$(i\omega_n - \varepsilon_{k'}) G_{kk'}(\omega_n, t') + a_o (\underline{A}\omega . \underline{k}') G_{kk'}(\omega_n - \omega_p, t')$$

$$+ \frac{J}{2N} \sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma^{\alpha}_{k\ell}(\omega_n, t') = \frac{i}{\beta} \delta_{kk'} e^{-\omega_n t'} \qquad (2.14)$$

The Fourier transform of the Dirac delta function is defined by

$$\delta(\omega_n, t') = + \frac{1}{-i\beta} \int_o^{-i\beta} \delta(t-t') e^{-\omega_n t} dt$$

$$= -\frac{1}{i\beta} e^{-\omega_n t'} \qquad \text{if } 0 > t' > -i\beta$$

$$= 0 \qquad \text{otherwise} \quad .$$

To obtain a closed set of equations, we must now write the equation of motion of $\Gamma^{\alpha}_{kk'}$. But this generates higher order Green's functions and the equations of motion of those generate still higher order Green's functions. In this way we obtain a chain of equations which cannot be solved. Hence one has to cut the chain by making some approximation. We shall come to this point later. Let us now write the equation of motion of $\Gamma^{\alpha}_{kk'}$: first of all we take

$$H = H_o + H^{\alpha}_{ex}$$

where we have not summed over the impurity position $\underline{R}\alpha$. The derivation of the equation follows as before. We have $< S^{\alpha}_z > = 0$, because there is no external magnetic field and so the impurity spins have no preferred direction. We obtain

$$i\frac{d\Gamma^{\alpha}_{kk'}(t,t')}{dt} = \delta(t-t')\langle [C_{k'\uparrow}S^{\alpha}_{z} + C_{k'\downarrow}S^{\alpha}_{-},\ C^{+}_{k\uparrow}]_{t=t'} \rangle$$

$$-i\langle Ti\frac{dC_{k'\uparrow}(t)}{dt} S^{\alpha}_{z}(t)C^{+}_{k\uparrow}(t') \rangle - i\langle TC_{k'\uparrow}(t)i\frac{dS^{\alpha}_{z}(t)}{dt} C^{+}_{k\uparrow}(t') \rangle$$

$$-i\langle Ti\frac{dC_{k'\downarrow}(t)}{dt} S^{\alpha}_{-}(t)C^{+}_{k\uparrow}(t') \rangle - i\langle TC_{k'\downarrow}(t)i\frac{dS^{\alpha}_{-}(t)}{dt} C^{+}_{k\uparrow}(t') \rangle \qquad (2.15)$$

We evaluate the commutators, $[C_k,H]$ etc., in (2.15) and use the following relations valid for $S^{\alpha} = \frac{1}{2}$:

$$S^{\alpha}_{\pm}S^{\alpha}_{z} = \mp \tfrac{1}{2}\ S^{\alpha}_{\pm}\ ,\quad S^{\alpha}_{z}S^{\alpha}_{\pm} = \pm \tfrac{1}{2}\ S^{\alpha}_{\pm}$$

and

$$S^{\alpha}_{+}S^{\alpha}_{-} = \tfrac{3}{4} + S^{\alpha}_{z} - (S^{\alpha}_{z})^{2}$$

Then Eq. (2.15) becomes

$$i\frac{d\Gamma^{\alpha}_{kk'}(t,t')}{dt} = \epsilon_{k'}(t)\Gamma^{\alpha}_{kk'}(t,t')$$

$$-\tfrac{3}{4}\frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha}G_{k\ell}(t,t')$$

$$-\frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha}\ \Gamma^{\alpha}_{k\ell}(t,t')$$

$$-i\frac{J}{2N}\sum_{\ell,\ell'} e^{i(\underline{\ell}'-\underline{\ell})\cdot\underline{R}\alpha}\langle TC_{k'\uparrow}(t)C^{+}_{\ell\uparrow}(t)C_{\ell'\downarrow}(t)S^{\alpha}_{-}(t)C^{+}_{k\uparrow}(t') \rangle$$

$$+i\frac{J}{2N}\sum_{\ell,\ell'} e^{i(\underline{\ell}'-\underline{\ell})\cdot\underline{R}\alpha}\langle TC_{k'\uparrow}(t)C^{+}_{\ell\downarrow}(t)C_{\ell'\uparrow}(t)S^{\alpha}_{+}(t)C^{+}_{k\uparrow}(t') \rangle$$

$$+i\frac{J}{2N}\sum_{\ell,\ell'} e^{i(\underline{\ell}'-\underline{\ell})\cdot\underline{R}\alpha}\langle TC_{k'\downarrow}(t)C^{+}_{\ell\uparrow}(t)C_{\ell'\uparrow}(t)S^{\alpha}_{-}(t)C^{+}_{k\uparrow}(t') \rangle$$

$$-i\frac{J}{2N}\sum_{\ell,\ell'} e^{i(\underline{\ell}'-\underline{\ell})\cdot\underline{R}\alpha}\langle TC_{k'\downarrow}(t)C^{+}_{\ell\downarrow}(t)C_{\ell'\downarrow}(t)S^{\alpha}_{-}(t)C^{+}_{k\uparrow}(t') \rangle$$

$$-i\frac{J}{N}\sum_{\ell,\ell'} e^{i(\underline{\ell}'-\underline{\ell})\cdot\underline{R}\alpha}\langle TC_{k'\downarrow}(t)C^{+}_{\ell\downarrow}(t)C_{\ell'\uparrow}(t)S^{\alpha}_{z}(t)C^{+}_{k\uparrow}(t') \rangle \qquad (2.16)$$

2.4 Decoupling Approximation

It can be seen in the last part of Eq.(2.16) that the Green's functions contain five operators. As mentioned before, the equations of these Green's functions generate still higher order Green's functions. Thus one is faced with a truly manybody problem to solve. At this point, one must make some approximation. We follow Nagaoka's decoupling scheme[49], where the average of some combination of operators is replaced by a product of averages of operators. In doing so, we combine the operators in such a manner that each average conserves spin. Lot of criticisms have been made of this approximation, but so far no substantial improvement could be achieved. One approach is to adopt what is called 'cumulant averages'[84]. But, whether this method provides any better approximation to this problem remains to be seen. Nagaoka[85], however, showed that his decoupling scheme is exact to infinite order of J as far as the most divergent logarithmic terms in each order of J are concerned.

We decouple the quantities that appear in Eq.(2.16) as follows:

$$< C_{k'\uparrow} C^{+}_{\ell\uparrow} C_{\ell'\downarrow} S^{\alpha}_{-} | C^{+}_{k\uparrow} > = < C_{k'\uparrow} C^{+}_{\ell\uparrow} > < C_{\ell'\downarrow} S^{\alpha}_{-} | C^{+}_{k\uparrow} >$$

$$+ < C^{+}_{\ell\uparrow} C_{\ell'\downarrow} S^{\alpha}_{-} > < C_{k'\uparrow} | C^{+}_{k\uparrow} >$$

$$< C_{k'\uparrow} C^{+}_{\ell\downarrow} C_{\ell'\uparrow} S^{\alpha}_{+} | C^{+}_{k\uparrow} >$$

$$= < C_{k'\uparrow} C^{+}_{\ell\downarrow} S^{\alpha}_{+} >< C_{\ell'\uparrow} | C^{+}_{k\uparrow} > + < C^{+}_{\ell\downarrow} C_{\ell'\uparrow} S^{\alpha}_{+} >< C_{k'\uparrow} | C^{+}_{k\uparrow} >$$

$$< C_{k'\downarrow}C^{+}_{\ell\uparrow}C_{\ell'\uparrow}S^{\alpha}_{-}|C^{+}_{k\uparrow} >$$

$$= < C^{+}_{\ell\uparrow}C_{\ell'\uparrow} >< C_{k'\downarrow}S^{\alpha}_{-}|C^{+}_{k\uparrow} > - < C^{+}_{\ell\uparrow}C_{k'\downarrow}S^{\alpha}_{-} >< C_{\ell'\uparrow}|C^{+}_{k\uparrow} >$$

$$< C_{k'\downarrow}C^{+}_{\ell\downarrow}C_{\ell'\downarrow}S^{\alpha}_{-}|C^{+}_{k\uparrow} >$$

$$= < C_{k'\downarrow}C^{+}_{\ell\downarrow} >< C_{\ell'\downarrow}S^{\alpha}_{-}|C^{+}_{k\uparrow} > + < C^{+}_{\ell\downarrow}C_{\ell'\downarrow} >< C_{k'\downarrow}S^{\alpha}_{-}|C^{+}_{k\uparrow} >$$

$$< C_{k'\downarrow}C^{+}_{\ell\downarrow}C_{\ell'\uparrow}S^{\alpha}_{z}|C^{+}_{k\uparrow} >$$

$$= < C_{k'\downarrow}C^{+}_{\ell\downarrow} >< C_{\ell'\uparrow}S^{\alpha}_{z}|C^{+}_{k\uparrow} > + < C_{k'\downarrow}C^{+}_{\ell\downarrow}S^{\alpha}_{z} >< C_{\ell'\uparrow}|C^{+}_{k\uparrow} >$$

(2.17)

where we denoted $< TA(t)B(t') >$ by $< A|B >$. We also use the following symmetry relations:

$$< C^{+}_{k\uparrow}C_{k'\uparrow} > = < C^{+}_{k\downarrow}C_{k'\downarrow} >$$

$$< C^{+}_{k\uparrow}C_{k'\downarrow}S^{\alpha}_{-} > = < C^{+}_{k\downarrow}C_{k'\uparrow}S^{\alpha}_{+} >$$

$$= 2< C^{+}_{k\uparrow}C_{k'\uparrow}S^{\alpha}_{z} > = -2< C^{+}_{k\downarrow}C_{k'\downarrow}S^{\alpha}_{z} >$$

(2.18)

2.5 Basic Equations in Electromagnetic Field

The Eq.(2.16) can then be written as

$$i\frac{d\Gamma^{\alpha}_{kk'}(t,t')}{dt} = \varepsilon_{k'}(t)\Gamma^{\alpha}_{kk'}(t,t') + \frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha}_{k\ell}(t,t')$$

$$- \tfrac{3}{4}\frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}G_{k\ell}(t,t')$$

$$- \frac{J}{N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}n^{\alpha}_{k'}(t)\Gamma^{\alpha}_{k\ell}(t,t')$$

$$+ \frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}m^{\alpha}_{k'}(t)G_{k\ell}(t,t')$$

(2.19)

where

$$n_k^\alpha(t) = \sum_\ell e^{i(\underline{k}-\underline{\ell})\cdot\underline{R}\alpha} < C^+_{\ell\uparrow}(t) C_{k\uparrow}(t) > \tag{2.20}$$

$$m_k^\alpha(t) = 3\sum_\ell e^{i(\underline{k}-\underline{\ell})\cdot\underline{R}\alpha} < C^+_{\ell\uparrow}(t) C_{k\downarrow}(t) S^\alpha_-(t) > \tag{2.21}$$

Now using the Fourier expansions of $G_{kk'}(t,t')$ and $\Gamma^\alpha_{kk'}(t,t')$ as before and the following Fourier transforms of the products,

$$\left[m^\alpha_{k'}(t) G_{k\ell}(t,t') \right]_{\omega_n,t'} \equiv \sum_{\omega_y} m^\alpha_{k'}(\omega_n-\omega_y) G_{k\ell}(\omega_y,t') \tag{2.22}$$

$$\left[n^\alpha_{k'}(t) \Gamma^\alpha_{k\ell}(t,t') \right]_{\omega_n,t'} \equiv \sum_{\omega_y} n^\alpha_{k'}(\omega_n-\omega_y) \Gamma^\alpha_{k\ell}(\omega_y,t') \tag{2.23}$$

the Eq.(2.19) reduces to

$$\begin{aligned}
&(i\omega_n-\varepsilon_{k'})\Gamma^\alpha_{kk'}(\omega_n,t') + a_o(\underline{A}\omega\cdot\underline{k}')\Gamma^\alpha_{kk'}(\omega_n-\omega_p,t') \\
&\quad + \tfrac{3}{4}\frac{J}{2N}\sum_\ell e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha} G_{k\ell}(\omega_n,t') \\
&\quad - \frac{J}{2N}\sum_\ell e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha}\Gamma^\alpha_{k\ell}(\omega_n,t') \\
&\quad + \frac{J}{N}\sum_\ell \left\{ e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha} \sum_{\omega_y} n^\alpha_{k'}(\omega_n-\omega_y)\Gamma^\alpha_{k\ell}(\omega_y,t') \right\} \\
&\quad - \frac{J}{2N}\sum_\ell \left\{ e^{i(\underline{\ell}-\underline{k}')\cdot\underline{R}\alpha} \sum_{\omega_y} m^\alpha_{k'}(\omega_n-\omega_y) G_{k\ell}(\omega_y,t') \right\} = 0
\end{aligned} \tag{2.24}$$

Next, we consider the remaining part of the Hamiltonian, i.e. $\sum_{\alpha' \neq \alpha} H_{ex}^{\alpha'}$. As S^{α} commutes with that part, it only comes in through the time derivative of $C_{k',\sigma}$ and we get the following terms

$$-i \sum_{\alpha' \neq \alpha} \sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha'} < TC_{\ell\uparrow}(t) S_z^{\alpha'}(t) S_z^{\alpha}(t) C_{k\uparrow}^{+}(t') >$$

$$-i \sum_{\alpha' \neq \alpha} \sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha'} < TC_{\ell\downarrow}(t) S_-^{\alpha'}(t) S_z^{\alpha}(t) C_{k\uparrow}^{+}(t') >$$

$$-i \sum_{\alpha' \neq \alpha} \sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha'} < TC_{\ell\downarrow}(t) S_z^{\alpha'}(t) S_-^{\alpha}(t) C_{k\uparrow}^{+}(t') >$$

$$+i \sum_{\alpha' \neq \alpha} \sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha'} < TC_{\ell\uparrow}(t) S_+^{\alpha'}(t) S_-^{\alpha}(t) C_{k\uparrow}^{+}(t') > \qquad (2.25)$$

Since we consider the case of very low concentration of impurities, we can neglect the interaction between the spins at different impurity sites. However, following Nagaoka[54] we take their effect into account by replacing $(i\omega_n - \varepsilon_{k'})$ appearing in (2.24) by $(i\Omega(\omega_n) - \varepsilon_{k'})$ where $\Omega(\omega_n)$ is a function of ω_n and is equal to ω_n in the lowest order approximation. Thus, the equation of motion for $\Gamma_{kk'}^{\alpha}$ can be written from Eq.(2.24) by replacing $(i\omega_n - \varepsilon_{k'})$ by $[i\Omega(\omega_n) - \varepsilon_{k'}]$, i.e. we write

$$\left[i\Omega(\omega_n) - \varepsilon_{k'}\right]\Gamma^{\alpha}_{kk'}(\omega_n,t') + a_o(\underline{A}\omega.\underline{k}')\Gamma^{\alpha}_{kk'}(\omega_n-\omega_p,t')$$

$$+ \tfrac{3}{4}\frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}(\omega_n,t')$$

$$- \frac{J}{2N}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha}_{k\ell}(\omega_n,t')$$

$$+ \frac{J}{N}\sum_{\ell}\left\{e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\sum_{\omega_y} n^{\alpha}_{k'}(\omega_n-\omega_y)\Gamma^{\alpha}_{k\ell}(\omega_y,t')\right\}$$

$$- \frac{J}{2N}\sum_{\ell}\left\{e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\sum_{\omega_y} m^{\alpha}_{k'}(\omega_n-\omega_y)G_{k\ell}(\omega_y,t')\right\} = 0 \qquad (2.26)$$

In the next chapter we solve the equations. There, we replace n^{α}_{k} and m^{α}_{k} by their impurity averaged quantities and then relate them to $\overline{G}_{kk'}$, $\overline{\Gamma}^{\alpha}_{kk'}$, which are also impurity averaged. These relations together with Eqs.(2.14) and (2.26) form a self-consistent closed set of equations.

CHAPTER 3 SOLUTIONS : CONDUCTIVITIES AT HIGH AND LOW TEMPERATURES

3.1 Introduction

Our aim has been to calculate the conductivity and hence the resistivity of the system from the response formalism so that we do not need to adopt the relaxation time approximation. The expectation value of the current operator is given by

$$< j_\mu(i\omega_p) > = < \rho_1(i\omega_p) j_\mu > \qquad (3.1)$$

where $\omega_p = 2\pi p/\beta$, $p = 0,\pm1,\pm2,\ldots$ are the Matsubara frequencies and ρ_1 is the first order correction to the density matrix. Eq.(3.1) gives rise to the familiar current-current correlation function[86] (Kubo formula) which can be related to the single particle Green's function of the system. However, there, we need to include the 'vertex corrections' that arise due to interference between the Green's functions[87], which occur while we average the product of two Green's functions in order to evaluate the current-current correlation function. This correction, to a certain approximation, is usually given by a complicated integral equation. Our purpose here to formulate the Green's function equations in the present manner is that if we calculate the single particle Green's function in the presence of a uniform field, this will give us the average current directly and the relevant corrections would be automatically taken into account. Although it is known[88] that the vertex corrections do not contribute to the conductivity of the system for s-wave scattering only, we

shall nevertheless show this explicitly so that the reader can follow easily the formulations of later chapters. We shall now solve the equations derived in the last chapter. As the response function, first order in the field, is sufficient to evaluate the transport properties, we shall consider equations relating to the first order terms only. We proceed in two steps. First we solve the equations formally when $\underset{\sim}{A}(t) = 0$ and then substitute the zeroth order terms from these solutions in the equations of the first order terms. Finally, we solve these equations.

3.2 Formal Solution in the Absence of the Field, $\underset{\sim}{A}(t) = 0$

When $\underset{\sim}{A}(t) = 0$, we can write

$$n_k^{\alpha}(\omega_n - \omega_y) = n_k^{\alpha_o} \delta_{\omega_n, \omega_y} \tag{3.2}$$

$$m_k^{\alpha}(\omega_n - \omega_y) = m_k^{\alpha_o} \delta_{\omega_n, \omega_y} \tag{3.3}$$

which implies that we now have a point interaction only at $\omega_n = \omega_y$. We also replace $m_k^{\alpha_o}$ and $n_k^{\alpha_o}$ by their impurity averaged values - which is a consistent approximation in the limit of small concentration of impurities. In terms of diagrams, this approximation is similar to ignoring the diagrams with crossing interaction lines in the calculation of $G_{kk'}^{(o)}$, that is, we write

$$\overline{n_k^{\alpha_o}} \equiv n_k^{(o)} \tag{3.4}$$

$$\overline{m_k^{\alpha_o}} \equiv m_k^{(o)} \tag{3.5}$$

Also, in the absence of the field, the Green's functions are functions of (t-t') only. Hence, we can drop the t' dependence. Then the Eqs.(2.14) and (2.26) reduce to

$$(i\omega_n - \varepsilon_{k'})G^{(o)}_{kk'}(\omega_n) + \frac{J}{2N}\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha_o}_{k\ell}(\omega_n) = \frac{i}{\beta}\delta_{kk'} \tag{3.6}$$

$$\left[i\Omega(\omega_n) - \varepsilon_{k'}\right]\Gamma^{\alpha_o}_{kk'}(\omega_n) + \frac{J}{N}\left(n^{(o)}_{k'} - \tfrac{1}{2}\right)\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha_o}_{k\ell}(\omega_n) - \frac{J}{2N}\left(m^{(o)}_{k'} - \tfrac{3}{4}\right)\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}G^{(o)}_{k\ell}(\omega_n) = 0 \tag{3.7}$$

We use zero suffix to indicate that the quantities are in the absence of the field. From Eq.(3.7) we find

$$\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha_o}_{k\ell}(\omega_n) = \frac{\frac{1}{2}J\Gamma(i\omega_n)}{1+JG(i\omega_n)}\sum_{\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}G^{(o)}_{k\ell}(\omega_n) \tag{3.8}$$

where

$$G(i\omega_n) = \frac{1}{N}\sum_{k}\frac{n^{(o)}_k - \frac{1}{2}}{[i\Omega(\omega_n) - \varepsilon_k]} \tag{3.9}$$

and

$$\Gamma(i\omega_n) = \frac{1}{N}\sum_{k}\frac{m^{(o)}_k - \frac{3}{4}}{[i\Omega(\omega_n) - \varepsilon_k]} \tag{3.10}$$

Substituting Eq.(3.8) in Eq.(3.6) and dividing both sides by $(i\omega_n - \varepsilon_{k'})$ we obtain

$$G^{(o)}_{kk'}(\omega_n) = \frac{i}{\beta}\frac{\delta_{kk'}}{(i\omega_n - \varepsilon_{k'})} + \frac{V'(i\omega n)}{(i\omega_n - \varepsilon_{k'})}\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}G^{(o)}_{k\ell}(\omega_n) \tag{3.11}$$

with

$$V'(i\omega_n) = -\frac{\frac{1}{4N}J^2\Gamma(i\omega_n)}{1 + JG(i\omega_n)} \tag{3.12}$$

Equation (3.11) is similar to the equation of ordinary potential scattering. This equation can be solved by the use of the technique of the multiple-scattering theory. When, $J = 0$, $V'(i\omega_n) = 0$ and we have a non-interacting system. The free electron propagator is given by

$$g_k(i\omega_n) = \frac{i}{\beta}\frac{1}{(i\omega_n - \varepsilon_k)} \tag{3.13}$$

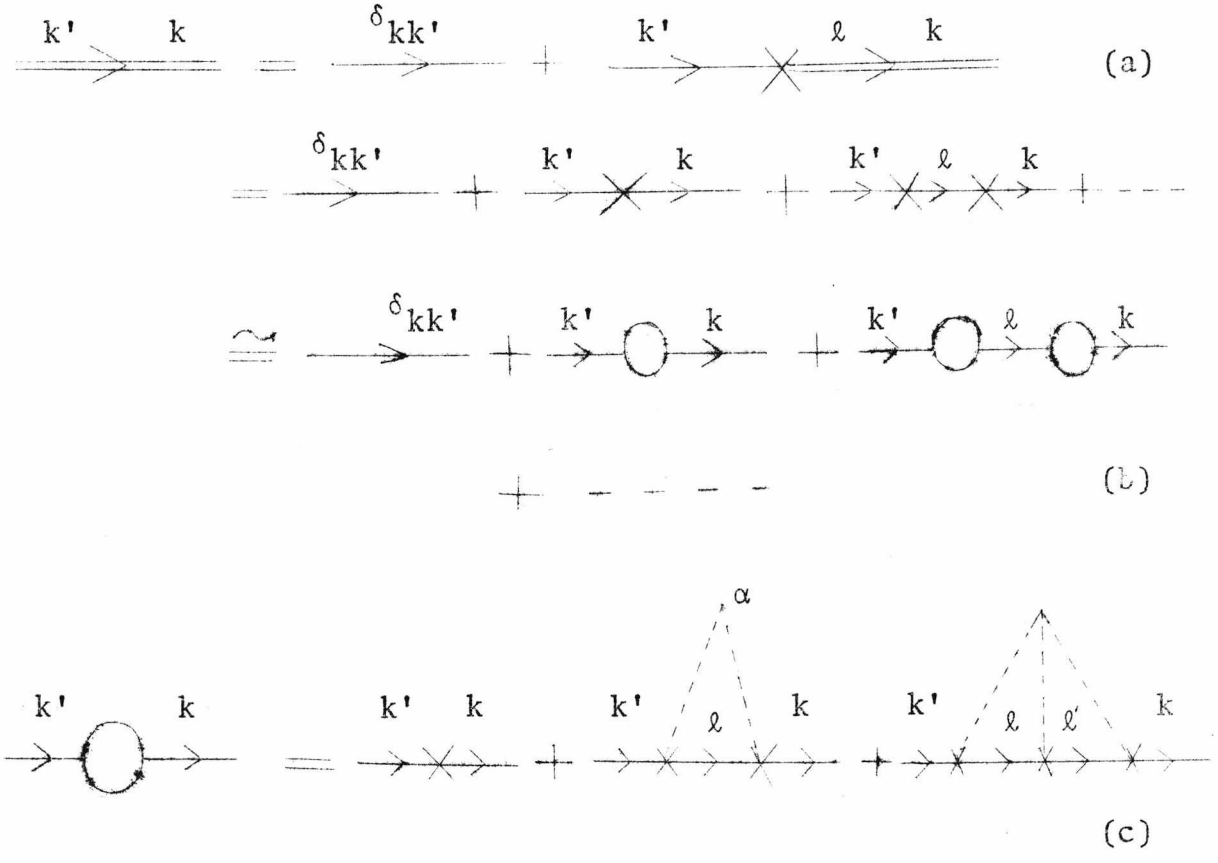
Then Eq.(3.11) can be written as

$$G^{(o)}_{kk'}(\omega_n) = g_{k'}\delta_{kk'} + V''(i\omega_n)g_{k'}\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}G^{(o)}_{k\ell}(\omega_n)$$

where

$$V''(i\omega_n) = -i\beta V'(i\omega_n) \tag{3.14}$$

Equation (3.14) is solved by the diagrammatic method. The solution is obtained as an infinite series as shown in Figure 2 where the double line indicates the single particle Green's function and the single line denotes the unperturbed Green's function, $g_k(i\omega_n)$. The cross denotes the interaction $V''(i\omega_n)$ with impurities.



(k',k are the momenta of the ingoing and outcoming electron lines)

Figure 2 : Calculation of $G^{(o)}_{kk'}(\omega_n)$. (b) shows expansion of $G^{(o)}_{kk'}(\omega_n)$; (c) shows an approximate evaluation of it.

For convenience, we join the crosses corresponding to the same impurity by dotted lines. Then typical fourth order terms in the expansion of Fig. 2(c) are:

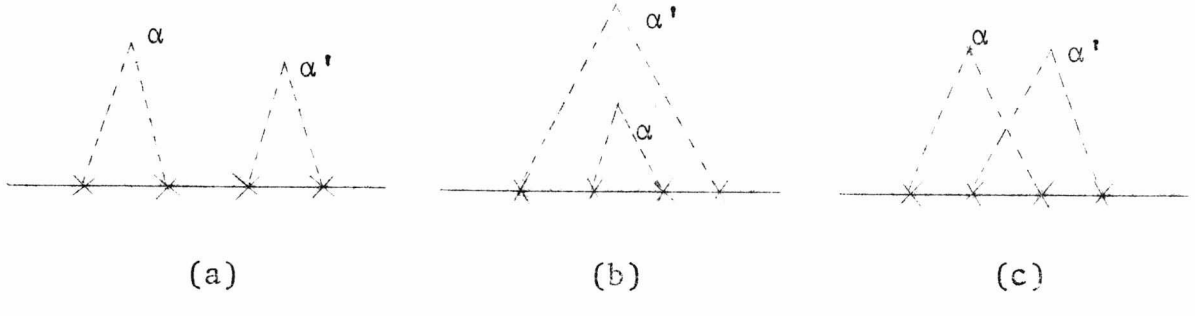


Figure 3 : The Fourth order diagrams

In the low density limit ($k_F \ell >> 1$ where ℓ is the electron mean free path) it can be shown that diagrams of the form Fig.3(c), with intersecting impurity lines are negligible. Thus, on summation of the series in Fig.2(c) we obtain

$$V'''(i\omega_n) = \frac{\frac{i\beta}{4N} J^2 \Gamma(i\omega_n)}{1 + JG(i\omega_n) + \frac{1}{4}J^2\Gamma(i\omega_n)F(i\omega_n)} \tag{3.15}$$

with

$$F(i\omega_n) = \frac{1}{N} \sum_k \frac{1}{[i\Omega(\omega_n) - \varepsilon_k]} \tag{3.16}$$

Finally, we average the equation of Fig.2(b) over the impurity positions and obtain

$$\overline{G^{(o)}_{kk'}}(\omega_n) = \frac{i}{\beta} \frac{\delta_{kk'}}{[i\omega_n - \varepsilon_k + V(i\omega_n)]} \tag{3.17}$$

with

$$V(i\omega_n) = \frac{\frac{1}{4}\frac{N_i}{N} J^2 \Gamma(i\omega_n)}{1 + JG(i\omega_n) + \frac{1}{4}J^2\Gamma(i\omega_n)F(i\omega_n)} \tag{3.18}$$

Now we recall the definitions of n_k^α and m_k^α from Eqs.(2.20) and (2.21). The impurity averaged quantities $n_k^{(o)}$ and $m_k^{(o)}$ are related to $\overline{G_k^{(o)}}(\omega_n)$ and $\overline{\Gamma^{\alpha o}}(\omega_n)$ in the following way

$$n_k^{(o)} = -i \sum_{\omega_n} \overline{G_k^{(o)}}(\omega_n) e^{i\omega_n 0+} \tag{3.19}$$

$$m_k^{(o)} = -2i \sum_{\omega_n} \overline{\Gamma_k^{\alpha o}}(\omega_n) e^{i\omega_n 0+} \tag{3.20}$$

The factor $e^{i\omega_n 0+}$, where 0+ is positive infinitesimal, ensures the convergence of the ω_n integral. To calculate $n_k^{(o)}$ and $m_k^{(o)}$ we must obtain $\bar{G}_k^{(o)}(\omega_n)$ and $\bar{\Gamma}_k^{\alpha o}(\omega_n)$ given by

$$\bar{G}_k^{(o)}(\omega_n) = \overline{\sum_{k'} e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} G_{k'k}^{(o)}(\omega_n)} \tag{3.21}$$

$$\bar{\Gamma}_k^{\alpha o}(\omega_n) = \overline{\sum_{k'} e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} \Gamma_{k'k}^{\alpha o}(\omega_n)} \tag{3.22}$$

$\bar{G}_k^{(o)}(\omega_n)$ can be calculated quite easily from the diagrammatic form of the Eq.(3.14). We multiply both sides by $V''(i\omega_n)e^{i(\underline{k}-\underline{k}').\underline{R}\alpha}$ and average over the impurity positions. This is illustrated in Fig.4. We have

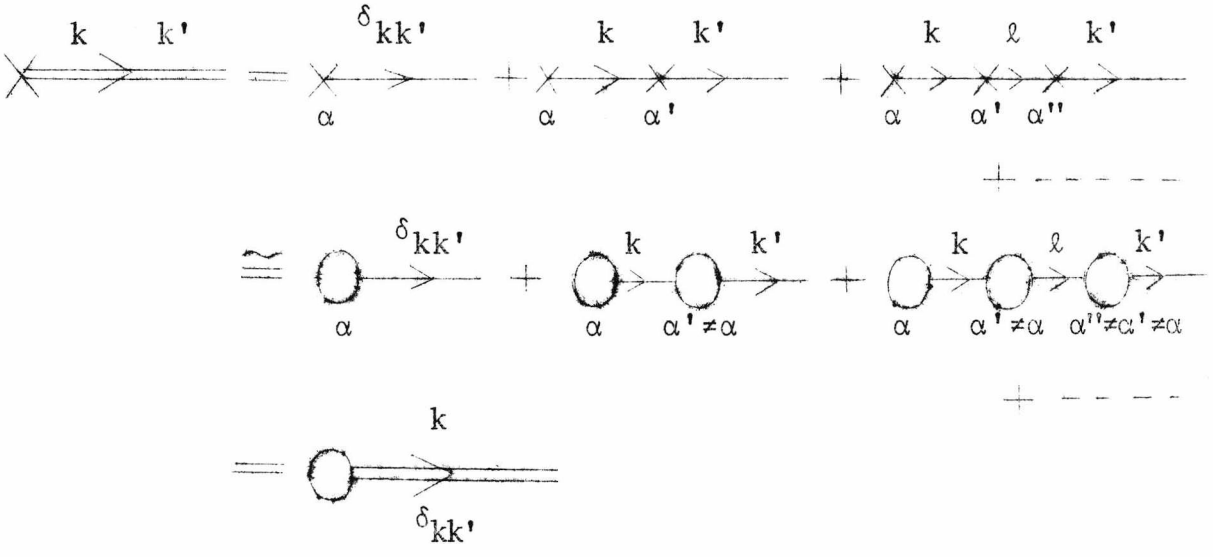


Figure 4 : Diagram illustrating the calculation of $\bar{G}_k^{(o)}(\omega_n)$.

$$V'(i\omega_n) \overline{\sum_{k'} e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} G^{(o)}_{k'k}} = V'''(i\omega_n)\overline{G^{(o)}_{kk}}$$

which gives

$$\overline{G}^{(o)}_k(\omega_n) = \frac{i}{\beta} \frac{1+JG(i\omega_n)}{1+JG(i\omega_n)+\frac{1}{4}J^2F(i\omega_n)\Gamma(i\omega_n)} \frac{1}{[i\omega_n - \varepsilon_k + V(i\omega_n)]} \tag{3.23}$$

$\overline{\Gamma}^{\alpha o}_k$ can be calculated from Eq.(3.7) by substituting Eq.(3.23). From Eq.(3.7) we obtain

$$\overline{\Gamma}^{\alpha o}_k(\omega_n) = \frac{J}{2N} \frac{(m^{(o)}_k-\frac{3}{4})[1+JG(i\omega_n)]-(n^{(o)}_k-\frac{1}{2})J\Gamma(i\omega_n)}{[i\Omega(\omega_n)-\varepsilon_k][1+JG(i\omega_n)]} \sum_\ell \overline{G}^{(o)}_\ell(\omega_n)$$

Using Eq.(3.23) we find

$$\overline{\Gamma}^{\alpha o}_k(\omega_n) = \frac{J}{2N} \frac{(m^{(o)}_k-\frac{3}{4})[1+JG(i\omega_n)]-(n^{(o)}_k-\frac{1}{2})J\Gamma(i\omega_n)}{[i\Omega(\omega_n)-\varepsilon_k][1+JG(i\omega_n)]} \frac{i}{\beta}\sum_\ell \frac{1}{[i\omega_n-\varepsilon_\ell+V(i\omega_n)]} \tag{3.24}$$

3.3 Formal Solution in the Presence of the Field

We now go back to the Eqns.(2.14) and (2.26) and consider the case when the external electromagnetic field $\underset{\sim}{A}(t)$ is not zero. We expand $G_{kk'}$, $\Gamma^{\alpha}_{kk'}$, n_k and m_k in terms of zero and one - where zero terms are values in the absence of the field and one terms are the terms of first order in the field. As mentioned before, we shall keep the first order terms in the field only. We write

$$G_{kk'}(\omega_n) = G^{(o)}_{kk'}(\omega_n) + G^{(1)}_{kk'}(\omega_n) \tag{3.25}$$

$$\Gamma^{\alpha}_{kk'}(\omega_n) = \Gamma^{\alpha o}_{kk'}(\omega_n) + \Gamma^{\alpha 1}_{kk'}(\omega_n) \tag{3.26}$$

$$n_k(\omega_n) = n^{(o)}_k(\omega_n) + n^{(1)}_k(\omega_n) \tag{3.27}$$

$$m_k(\omega_n) = m^{(o)}_k(\omega_n) + m^{(1)}_k(\omega_n) \tag{3.28}$$

We consider the response at a single frequency, i.e. the field is of the form, $\underset{\sim}{A}(t) = \underset{\sim}{A}_{\omega} e^{-i\omega t}$ and we had set $-i\omega = \omega_p$. Since $n^{(1)}_k(\omega_n)$ and $m^{(1)}_k(\omega_n)$ are first order in the field, we can write

$$n^{\alpha 1}_k(\omega_n) = n^{\alpha 1}_k \, \delta_{\omega_p, \omega_n} \tag{3.29}$$

$$m^{\alpha 1}_k(\omega_n) = m^{\alpha 1}_k \, \delta_{\omega_p, \omega_n} \tag{3.30}$$

Substitution of Eqs.(3.25) to (3.30) in Eqs.(2.14) and (2.26) and collection of the first order terms yield

$$(i\omega_n - \varepsilon_{k'}) G^{(1)}_{kk'}(\omega_n, t') + a_o(\underset{\sim}{A}_{\omega} \cdot \underline{k}') G^{(o)}_{kk'}(\omega_n - \omega_p, t')$$

$$+ \frac{J}{2N} \sum_{\ell, \alpha} e^{i(\underline{\ell} - \underline{k}') \cdot \underline{R}\alpha} \Gamma^{\alpha 1}_{k\ell}(\omega_n, t') = 0 \tag{3.31}$$

$$[i\Omega(\omega_n)-\epsilon_{k'}]\Gamma^{\alpha 1}_{kk'}(\omega_n,t') + a_o(\underset{\sim}{A}_\omega.\underset{\sim}{k}')\Gamma^{\alpha o}_{kk'}(\omega_n-\omega_p,t')$$

$$+ \frac{J}{N}\left(n^{(o)}_{k'}-\tfrac{1}{2}\right)\sum_{\ell} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}\Gamma^{\alpha 1}_{k\ell}(\omega_n,t')$$

$$- \frac{J}{2N}\left(m^{(o)}_{k'}-\tfrac{3}{4}\right)\sum_{\ell} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}G^{(1)}_{k\ell}(\omega_n,t')$$

$$+ \frac{J}{N} n^{(1)}_{k'} \sum_{\ell} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}\Gamma^{\alpha o}_{k\ell}(\omega_n-\omega_p,t')$$

$$- \frac{J}{2N} m^{(1)}_{k'} \sum_{\ell} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}G^{(o)}_{k\ell}(\omega_n-\omega_p,t') = 0 \qquad (3.32)$$

Now, we eliminate $\Gamma^{\alpha 1}_{kk'}$ from Eq.(3.31) by substituting its value from Eq.(3.32). We have, from Eq. (3.32)

$$\sum_{\ell,\alpha} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}\Gamma^{\alpha 1}_{k\ell}(\omega_n,t') = -\sum_{\ell,\alpha}\frac{a_o(\underset{\sim}{A}_\omega.\underset{\sim}{\ell})}{(i\omega_n-\epsilon_\ell)} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}\Gamma^{\alpha o}_{k\ell}(\omega_n-\omega_p,t')$$

$$- JG(i\omega_n)\sum_{\ell,\alpha} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}\Gamma^{\alpha 1}_{k\ell}(\omega_n,t')$$

$$+ \tfrac{1}{2}J\Gamma(i\omega_n)\sum_{\ell,\alpha} e^{i(\underset{\sim}{\ell}-\underset{\sim}{k}').\underset{\sim}{R}\alpha}G^{(1)}_{k\ell}(\omega_n,t') \qquad (3.33)$$

Here, the two terms containing $m^{(1)}_k$ and $n^{(1)}_k$ vanished - since these quantities are first order in the field, they must occur in the form $(\underset{\sim}{A}\omega.\underset{\sim}{k})$ and hence angular integrations of the k-sum would give zero. By substituting for $\Gamma^{\alpha o}_{kk'}$ from Eq.(3.7) in the first term of the r.h.s. of Eq.(3.33), one can also show that this term vanishes. Hence, we have,

from Eq.(3.33)

$$\sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma_{k\ell}^{\alpha 1}(\omega_n,t') = \frac{\frac{1}{2}J\Gamma(i\omega_n)}{1+JG(i\omega_n)} \sum_{\ell,\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}^{(1)}(\omega_n,t') \tag{3.34}$$

Substitution of Eq.(3.34) in Eq.(3.31) yields

$$G_{kk'}^{(1)}(\omega_n,t') = i\beta g_{k'} a_o(\underline{A}\omega.\underline{k}') G_{kk'}^{(o)}(\omega_n - \omega_p,t') - i\beta g_{k'} V'(i\omega_n) \sum_{\ell} \sum_{\alpha} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}^{(1)}(\omega_n,t') \tag{3.35}$$

with g_k and $V'(i\omega_n)$ as defined before in Eqs.(3.13) and (3.12).

We solve Eq.(3.35) using similar diagrammatic technique as before. We illustrate this in Figure 5.

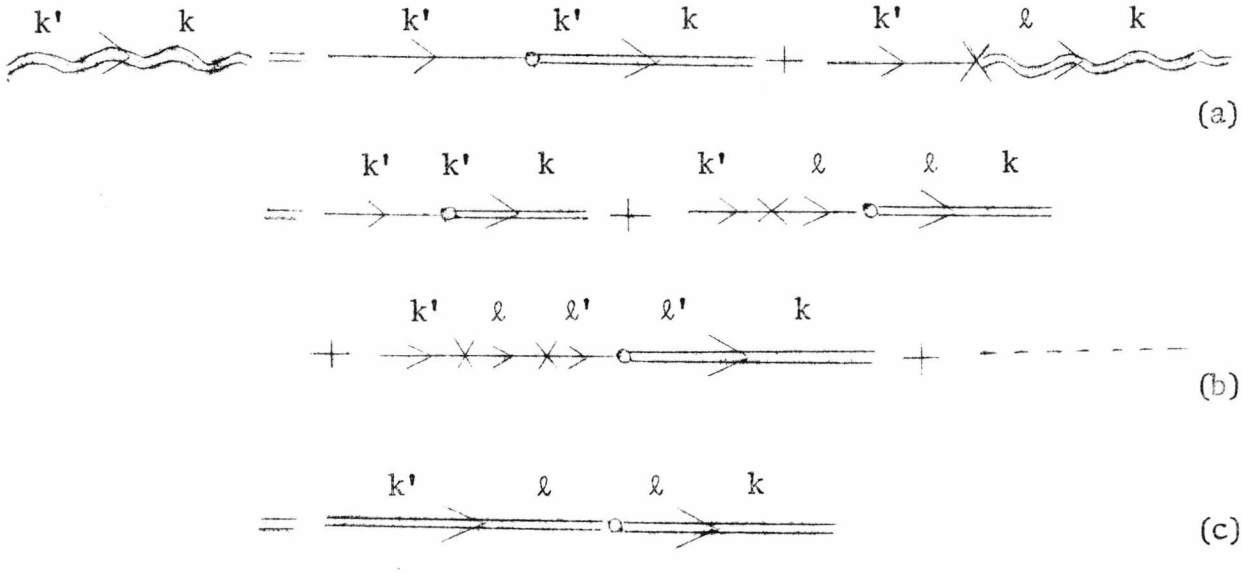


Figure 5 : Calculation of $G_{kk'}^{(1)}$ denoted by wavy double lines.

In averaging over the impurity positions in Figs.5(b), 5(c), we neglected averaging across the vertex. It can be seen quite easily that this averaging does not contribute to $G^{(1)}_{kk'}$ for our point interaction formulation. The phase factor associated with the interaction potential is independent of the dummy variable, ℓ and hence when summed over, the higher order terms in the typical 'ladder sum' would vanish due to angular integrations. This, in fact,is due to the fact that momentum has to be conserved at each impurity site when averaged over the impurity positions. We can see this clearly from a typical term arising in the expansion of $G^{(1)}_{kk'}$, (Fig. 6).

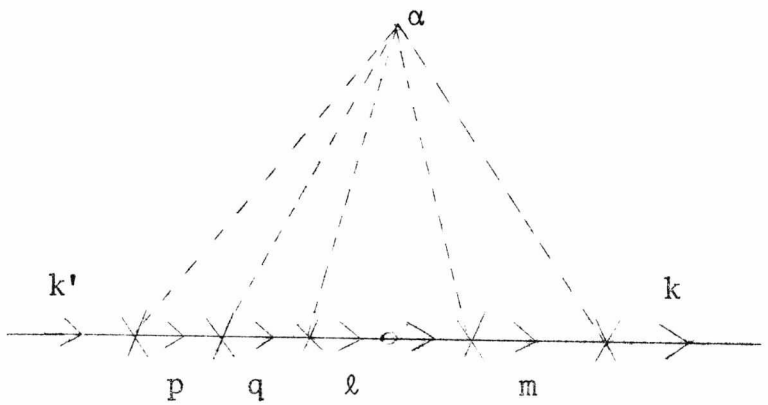


Figure 6 : Averaging over the impurity site across the vertex.

Contribution from Fig. 6 can be written as

$$[-V'(i\omega_n)]^5(i\beta)^5 \sum_{\substack{p,q,\ell \\ m}} a_o(\underline{A}\omega.\underline{\ell})\, g_p g_q g_\ell g_m e^{i(\underline{p}-\underline{k}').\underline{R}\alpha+i(\underline{q}-\underline{p}).\underline{R}\alpha+i(\underline{\ell}-\underline{q}).\underline{R}\alpha}$$

$$\cdot\, e^{i(\underline{m}-\underline{\ell}).\underline{R}\alpha+i(\underline{k}-\underline{m}).\underline{R}\alpha}$$

$$=[-V'(i\omega_n)]^5(i\beta)^5 \sum_{\substack{p,q,\ell \\ m}} a_o(\underline{A}\omega.\underline{\ell}) g_p g_q g_\ell g_m e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} = 0$$

Because the angular integral in the ℓ sum gives zero.

As we know $G^{(1)}_{kk'}$ gives average current directly through a relation

$$< J > = J_o \sum_{k,\omega_n} \underline{k}\bar{G}^{(1)}_{kk}(\omega_n) \qquad (3.35)$$

we can insert another $\underline{k}$ vertex in each term in the series for $G^{(1)}_{kk'}$ and calculate the average current. This is shown in diagram 7.

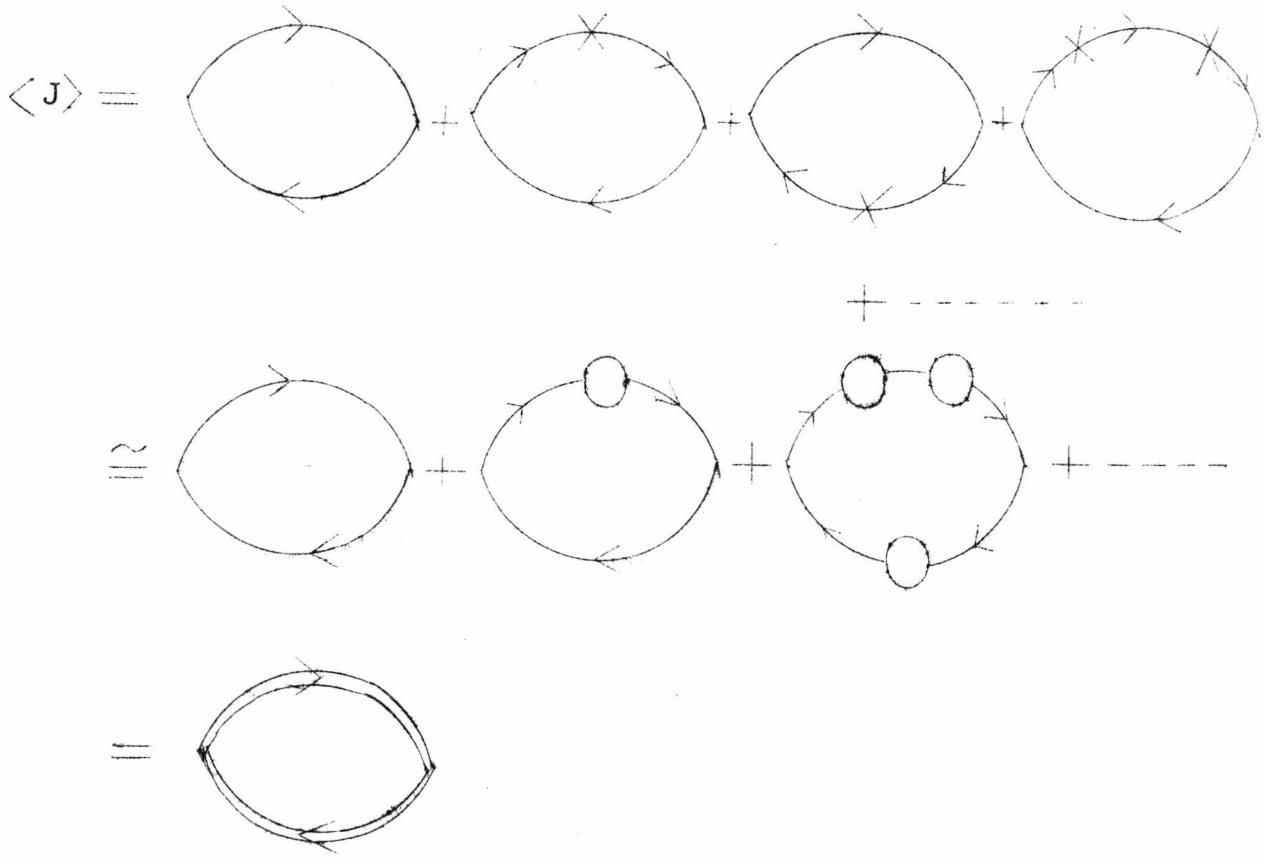


Figure 7 : Diagrams to calculate the average current < J > .

The current is given by (Fig.7)

$$J_\mu = \beta v A_\nu \left(\frac{e}{m^* v}\right)^2 \sum_{k,\omega_n} k_\mu k_\nu \bar{G}^{(o)}_{kk}(\omega_n)\bar{G}^{(o)}_{kk}(\omega_n-\omega_p) \qquad (3.36)$$

where v is the volume of the crystal and all other quantities are already defined.

3.4 Conductivity at High Temperatures, $T > T_k$.

By high temperatures, we mean, temperature greater than the Kondo temperature, T_k, where the perturbation series diverges. In Nagaoka formulation this is the critical temperature, T_c. We can replace $n_k^{(o)}$ and $m_k^{(o)}$ by their zeroth-order quantities with respect to J. Thus, we have

$$m_k^{(o)} = 0 \ , \ n_k^{(o)} = f_k = f(\varepsilon_k) \tag{3.37}$$

Then, in the lowest order approximation

$$F(i\omega_n) = - \frac{i\pi\rho}{N} \text{ sign } \omega_n \tag{3.38}$$

$$\Gamma(i\omega_n) = i\frac{3}{4N}\pi\rho \text{ sign } \omega_n \tag{3.39}$$

and

$$G(i\omega_n) = \frac{\rho}{2N} \int_{-D}^{D} \frac{1}{(\varepsilon - i\omega_n)} \tanh\left(\frac{\varepsilon}{2T}\right) d\varepsilon \tag{3.40}$$

where ρ is the density of states of conduction electrons of pure metal near the Fermi surface and we introduced the cut-off parameter D in the ε integral as the integral diverges as $\varepsilon \to \infty$. We approximate (3.40) at T = 0 which is, more or less, a standard technique and obtain

$$G(i\omega_n) = -\frac{\rho}{N} \ln\left|\frac{\omega_n}{D}\right| \quad \text{for } D >> \omega_n \tag{3.40a}$$

Then, using Eqs.(3.38), (3.39) and (3.40a) in Eq.(3.18) we get

$$V(i\omega_n) \cong \frac{i\frac{3}{16N}c\pi\rho J^2 \text{sign } \omega_n}{1-\frac{\rho J}{N}\ell n\left|\frac{\omega_n}{D}\right|} \equiv if(\omega_n)\text{sign } \omega_n \qquad (3.41)$$

where, we neglected the J^2 term in the denominator because it is small compared to 1. Also, we put $c = Ni/N$, the concentration of impurities. From Eqs.(3.41), (3.17) and (3.36), we obtain

$$J_\mu = -\frac{v}{3\beta}\left(\frac{e}{m^*v}\right)^2 A_\mu \rho k_F^2 \sum_{\omega_n} \int_{-D}^{D} \frac{d\varepsilon}{[\varepsilon - i\omega_n - V(i\omega_n)][\varepsilon - i\omega_n - i\omega_p - V(i\omega_n + i\omega_p)]} \qquad (3.42)$$

where k_F is the momentum of the conduction electron at the Fermi surface and, ρ is the density of states for both spins ($= 3N/2\varepsilon_F$). For convenience, we changed the variable $\omega_n - \omega_p$ to ω_n' and relabelled ω_n. The ε-integral now converges as $\varepsilon \to \infty$ and we can extend the limits to ∞ to $-\infty$. Then the integral is easily performed around the contour as shown in Fig.8. Then we get

$$J_\mu = -\frac{2\pi v}{3\beta}\left(\frac{e}{m^*v}\right)^2 A_\mu \rho k_F^2 \xi(\omega_p) \qquad (3.43)$$

where

$$\xi(\omega_p) = \sum_{-\omega_p < \omega_n < 0} \frac{1}{\omega_p + \frac{\gamma}{1 - b\,\ell n \frac{\omega_n + \omega_p}{D}} + \frac{\gamma}{1 - b\,\ell n \frac{-\omega_n}{D}}} \qquad (3.44)$$

with

$$\gamma = \frac{3}{16}\frac{N_i}{N^2}\pi\rho J^2 \quad , \quad b = \frac{\rho J}{N} \tag{3.45}$$

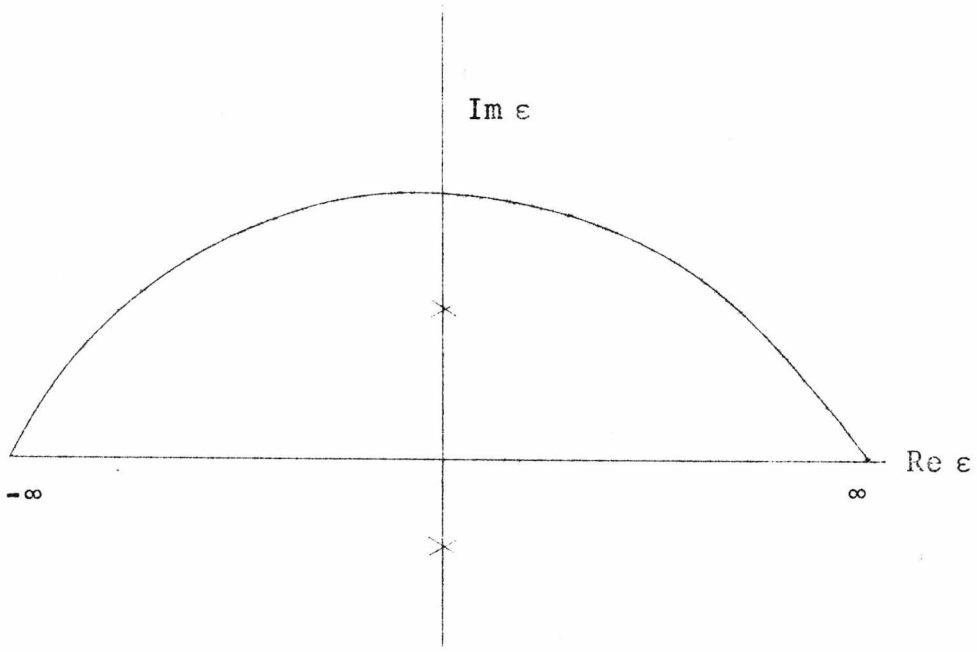


Figure 8 : The contour of the ε-integral.

Next, we have to perform the ω_n sum in the restricted region. This can be done by transforming the ω_n sum to a contour integral using the relation

$$\sum_{\omega_n} f(\omega_n) = \frac{-\beta}{2\pi i}\int_{c'} \frac{dz}{e^{\beta z}+1} f(-iz) \tag{3.46}$$

The integrand has poles along Im z-axis at $z = i\omega_n$ and the contour c' encloses them. The appropriate contour c' for the ω_n sum is shown in Figure 9.

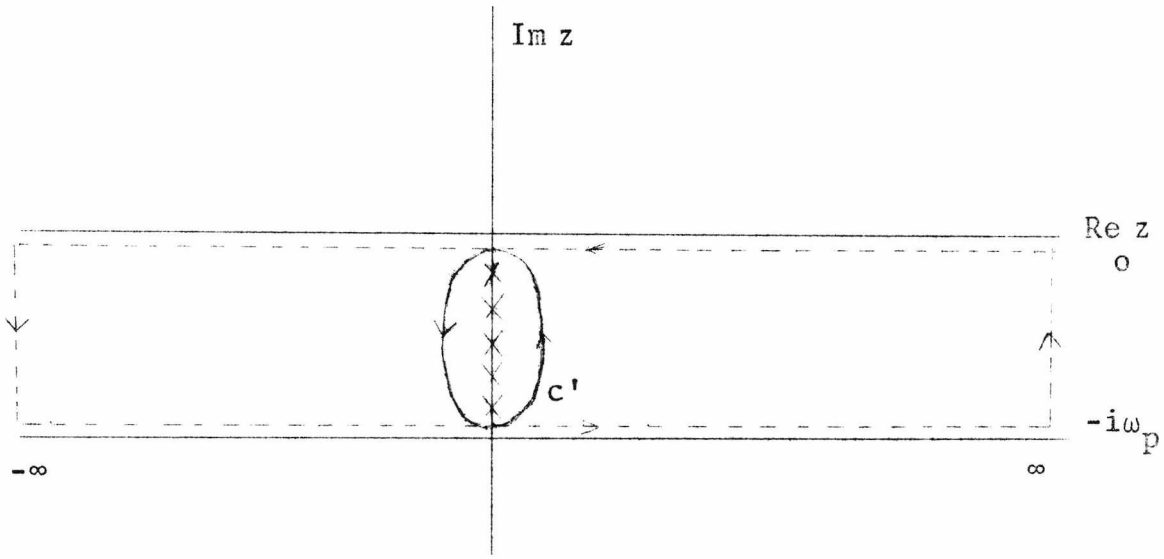


Figure 9 : Contour in the complex plane for summing over the Fourier energies.

We can now deform the contour as shown in Fig.9 and integrate along the dashed lines.† We obtain

$$\xi(\omega_p) = \frac{\beta}{2\pi i}\int \frac{dz}{e^{\beta z}+1} \frac{1}{\omega_p + \dfrac{\gamma}{1 - b\ell n\dfrac{-iz+\omega_p}{D}} + \dfrac{\gamma}{1 - b\ell n\dfrac{iz}{D}}}$$

$$- \frac{\beta}{2\pi i}\int \frac{dz}{e^{\beta z}+1} \frac{1}{\omega_p + \dfrac{\gamma}{1 - b\ n\dfrac{-iz}{D}} + \dfrac{\gamma}{1 - b\ n\dfrac{iz+\omega_p}{D}}} \qquad (3.47)$$

At this stage, we can make analytic continuation to real frequencies, $i\omega_p \to \omega + i0+$, which gives

† There are two points to be cleared up: (i) one has to show that the contributions from the end-bits of the contour vanish, (ii) that there are no poles in the deformed region. These are done in the Appendix A.

$$\xi(-i\omega) = \frac{\beta}{2\pi i}\int f(x)dx\left\{\frac{1}{-i\omega + \dfrac{\gamma}{1 - b\,\ell n\dfrac{-i\omega-ix}{D}} + \dfrac{\gamma}{1 - b\ell n\dfrac{ix}{D}}}\right.$$

$$\left. - \frac{1}{-i\omega + \dfrac{\gamma}{1 - b\ell n\dfrac{-ix}{D}} + \dfrac{\gamma}{1 - b\ n\dfrac{ix-i\omega}{D}}}\right\} \qquad (3.48)$$

where f(x) is the Fermi function. Eq.(3.48) can be written as

$$\xi(-i\omega) = \frac{\beta}{2\pi i}\int f(x)dx\Big\{\phi(x) - \phi(x-\omega)\Big\} \qquad (3.49)$$

where

$$\phi(x) = \frac{1}{-i\omega + \dfrac{\gamma}{1 - b\ell n\dfrac{ix}{D}} + \dfrac{\gamma}{1 - b\ n\dfrac{-ix-i\omega}{D}}} \qquad (3.50)$$

We change the variable x-ω to x' in the second term of Eq.(3.49) and relabel x, to obtain

$$\xi(-i\omega) = \frac{\beta}{2\pi i}\int\phi(x)[f(x) - f(x+\omega)]dx$$

$$\cong -\frac{i\omega\beta}{2\pi}\int\phi(x)\Big/_{\omega=0}\left[-\frac{\partial f(x)}{\partial x}\right]dx \qquad (3.51)$$

Expanding in powers of J, which is consistent at high temperatures, one obtains

$$\phi(x)\Big|_{\omega=0} \cong \frac{1}{2\gamma}\left[1 - b\ell n\left|\frac{x}{D}\right|\right] \tag{3.52}$$

Substituting Eq. (3.52) in Eq. (3.51) and performing the x-integral one obtains

$$\xi(-i\omega) = -\frac{i\omega\beta}{2\pi}\frac{1}{2\gamma}\left[1 - b\ell n\left|\frac{T}{1.13D}\right|\right] \tag{3.53}$$

Thus, using Eqs.(3.53), (3.45), the current is found to be

$$J_\mu = i\omega A_\mu \frac{1}{3}\frac{e^2}{m^{*2}v}\rho k_F^2 \frac{16N}{3\pi\rho cJ^2}\left[1 - \frac{\rho J}{N}\ell n\left|\frac{T}{1.13D}\right|\right] \tag{3.54}$$

The d.c. conductivity σ , for $J < 0$ is given by

$$\sigma = \frac{1}{2}\frac{ne^2}{m^*}\frac{16N}{3\pi\rho cJ^2}\left[1 + \frac{\rho|J|}{N}\ell n\left|\frac{T}{1.13D}\right|\right] \tag{3.55}$$

This is essentially the Kondo result as obtained by Nagaoka. Our result differs from Nagaoka by an overall factor $\frac{1}{2}$ and 0.68 in the ℓn term. Nagaoka's formula (5.3) agrees with ours, which is derived from the current-current correlation function, for the free electron gas. But his definition, $\tau_k^{-1} = -\text{Im}\, G_{kk}^{-1}(-i\omega)$ has to be replaced by $(2\tau_k)^{-1} = -\text{Im}G_{kk}^{-1}(-i\omega)$ to account for the factor $\frac{1}{2}$ in our result. Furthermore, Nagaoka used his expression (3.9) for evaluating his (5.5) rather than using his (3.10). This

will account for the factor appearing inside the ℓn.

Thus, we see although we adopted a different method to calculate the conductivity of a Kondo system, we arrived at the same result. This substantiates the belief that the metallic systems containing a very dilute concentration of paramagnetic impurities can be treated, to a reasonable approximation, as though it relaxes with a characteristic time τ .

3.5 Conductivity at Low Temperatures, $T < T_k$.

At low temperatures, a straightforward perturbation expansion is not possible. The $m_k^{(o)}$ is then expected to be large near $\varepsilon_k = 0$. We shall follow Nagaoka procedure to find a solution at low temperatures, valid near the Fermi surface. We shall solve for the case $J < 0$.

Let us assume,

$$(m_k^{(o)} - \tfrac{3}{4}) = \alpha(n_k^{(o)} - \tfrac{1}{2})/\varepsilon_k \qquad (3.56)$$

where, $\alpha > o$, is a parameter to be determined self consistently. Then $G(i\omega_n)$ becomes

$$G(i\omega_n) = \frac{i\omega_n}{\alpha}\Gamma(i\omega_n) - \frac{1}{N}\sum_k \frac{n_k - \frac{1}{2}}{\varepsilon_k} \qquad (3.57)$$

Then, substituting (3.57) in (3.18) one finds

$$V(i\omega_n) = if(\omega_n)\,\text{sign}\,\omega_n$$

where

$$f(\omega_n) = \frac{\gamma'}{|\omega_n| + \Delta} \quad \text{and} \quad \gamma' = \tfrac{1}{4}c|J|\alpha\,, \quad \Delta = \alpha|J|\rho\pi/4N \qquad (3.58)$$

provided,

$$1 + \frac{|J|}{N} \sum_k \frac{n_k - \frac{1}{2}}{\varepsilon_k} = 0 \qquad (3.59)$$

Δ depends on α and, has to be determined self-consistently from the Eq.(3.59). Then the expression for average current is given by, as before,

$$J_\mu = -\frac{1}{3\beta} \frac{e^2}{m^{*2}v} A_\mu \rho k_F^2 \sum_{\omega_n} \int \frac{d\varepsilon}{[\varepsilon - i\omega_n - V(i\omega_n)][\varepsilon - i\omega_n - i\omega_p - V(i\omega_n + i\omega_p)]}$$

Performing the ε-integral, one obtains

$$J_\mu = -\frac{2\pi}{3\beta} \frac{e^2}{m^{*2}v} A_\mu k_F^2 \rho \; \xi(\omega_p)$$

where

$$\xi(\omega_p) = \sum_{-\omega_p < \omega_n < 0} \frac{1}{\omega_p + \frac{\gamma'}{\Delta - \omega_n} + \frac{\gamma'}{\Delta + \omega_n + \omega_p}} \qquad (3.60)$$

The ω_n sum follows exactly the same way as before and after making analytic continuation, we obtain

$$\xi(-i\omega) = \frac{\beta}{2\pi i} \int f(x) \left[\phi(x) - \phi(x-\omega) \right] \qquad (3.61)$$

with

$$\phi(x) = \frac{1}{-i\omega + \frac{\gamma'}{\Delta + ix} + \frac{\gamma'}{\Delta - ix - i\omega}} \qquad (3.62)$$

Again, in the d.c. limit

$$\xi(-i\omega) = -\frac{i\omega\beta}{2\pi}\int \frac{1}{\frac{\gamma'}{\Delta + ix} + \frac{\gamma'}{\Delta - ix}} \left(-\frac{\partial f}{\partial x}\right) dx$$

which gives

$$\xi(-i\omega) = -\frac{i\omega\beta}{2\pi}\,\frac{\Delta}{2\gamma'}\left[1 + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2\right] \tag{3.63}$$

Then using Eqs.(3.58) and (3.60) the conductivity is obtained as

$$\sigma = \frac{ne^2}{m^*}\,\frac{\pi\rho}{2cN}\left[1 + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2\right] \tag{3.64}$$

A factor of 2 can be taken into account in the same way as before. Eq.(3.64) gives the low temperature conductivity of Kondo alloys and this goes to a constant as $T \to 0$.

Now, one has to determine the temperature dependence of the function Δ from Eq.(3.59). This has been done by Nagaoka and we shall not persue this point any further, but quote Nagaoka's result. For two limiting concentrations of impurities Δ's are obtained to be, at $T = 0$

$$\Delta = \Delta_o - \frac{cN}{2\pi\rho} \qquad \text{for } c << \frac{\rho}{N}\Delta_o$$

$$= \frac{\pi\rho}{cN}\Delta_o^2 \qquad \text{for } c >> \frac{\rho}{N}\Delta_o$$

where

$$\Delta_o = D \exp[- N/|J|\rho] \quad .$$

For higher temperatures, the approximate solutions give, for $T \sim 0$,

$$\Delta(T) = \Delta(0)[1 - AT^2]$$

where

$$A = \frac{\pi^2}{6} \frac{1}{\Delta_o^2} \left[1 - \frac{9}{4} \frac{c}{\pi\rho\Delta_o} \right] \qquad \text{for } c << \frac{\rho}{N} \Delta_o$$

$$= \frac{\pi^2}{6} \frac{1}{\Delta_o^2} \left[1 - \frac{\pi\rho\Delta_o}{2cN} \right] \qquad \text{for } c >> \frac{\rho}{N} \Delta_o$$

and for $T \lesssim T_c$

$$\Delta(T) \simeq \frac{4}{\pi} (T_c - T) \quad .$$

with

$$T_c = 1.14D \exp(N/J\rho) \quad .$$

CHAPTER 4 THE A.C. CONDUCTIVITY AT LOW TEMPERATURES

4.1 Introduction

In the last chapter, we applied linear response formalism to the Kondo problem. For contact interaction, we found that 'the vertex corrections' dropped out and the conductivity could be calculated from the current-current correlation function in a straightforward manner. In that case, the transport relaxation time reduces to ordinary relaxation time for the scattering of conduction electrons by the impurities. As a result of applying the response formalism, we have succeeded in calculating analytically the frequency dependent conductivity (valid for $\omega << \omega_{max} \sim 10^{12}$Hz) at low temperatures.

Although there exist a few theoretical calculations of frequency-dependent conductivity of the Kondo system, there are hardly any experimental data available to compare. Kakitani[89] has carried out a perturbational calculation of the complex conductivity, $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$, based on the s-d exchange model valid at temperatures higher than the Kondo temperature, T_k. Calculations by Moriya and Inoue[90] of the frequency dependent conductivity of a dilute magnetic alloy have indicated that measurements of the surface resistance of a Kondo alloy in the microwave or far infrared region might distinguish between the s-d and ℓsf (localised spin fluctuation) models. Their results indicate significant deviation from the Drude model and predict a peak at finite frequencies in the real part of the conductivity. Murata and Wilkins[91] calculated the surface

resistance of Kondo alloys by solving the t-matrix of the s-d model numerically. They also have suggested that a peak might be observed in the frequency dependent conductivity. But, the experimental data[92] so far available have not supported this prediction.

Our analytic expressions do not show any peak in the real part of the conductivity. But, since our calculations are valid at low frequencies and low temperatures, we are not in a position to draw any definite conclusion. We shall discuss this point in the last section of this chapter.

4.2 Frequency-Dependent Conductivity at Absolute Zero Temperature.

Let us recall the expression for average current at low temperatures:

$$j_\mu = -\frac{2\pi}{3\beta}\frac{e^2}{m^{*2}v} A_\mu k_F^2 \rho \; \xi(\omega_p) \tag{4.1}$$

where

$$\xi(\omega_p) = \sum_{-\omega_p < \omega_n < 0} \frac{1}{\omega_p + \frac{\gamma'}{\Delta - \omega_n} + \frac{\gamma'}{\Delta + \omega_n + \omega_p}} \tag{4.2}$$

with

$$\gamma' = \tfrac{1}{4} c|J|\alpha \qquad \text{and} \qquad \Delta = \alpha|J|\rho\pi/4N \tag{4.3}$$

The ω_n sum now has to be performed carefully, since we are not interested in the d.c. conductivity any more but want to extend it to all frequencies. We notice that the summand in Eq.(4.2) goes as ω_p^{-1} as $\omega_n \to \infty$. So if we subtract ω_p^{-1}

from the summand at the outset, the summand will be absolutely convergent as $\omega_n \to \infty$ and the contributions from the end parts of the contour (Fig.9) will pose no problem. Then, transforming the ω_n sum to the contour integral form we arrive at the following expression:

$$\xi(-i\omega) = \frac{\beta}{2\pi} - \frac{\beta}{2\pi i}\int \frac{dx}{e^{\beta x}+1}\left\{\frac{1}{-i\omega + \frac{\gamma'}{\Delta - ix} + \frac{\gamma'}{\Delta + ix - i\omega}}\right.$$

$$\left. - \frac{1}{-i\omega + \frac{\gamma'}{\Delta + ix} + \frac{\gamma'}{\Delta - ix - i\omega}}\right\} \qquad (4.4)$$

where we already made the analytic continuation to the real frequencies. We write the expression (4.4) in the following form

$$\xi(-i\omega) = \frac{\beta}{2\pi} - \frac{\beta}{2\pi i}\int \frac{dx}{e^{\beta x}+1}\, g(x) \qquad (4.5)$$

where

$$g(x) = \frac{c_1}{ax^2 - bx + c_2} - \frac{c_1}{ax^2 + bx + c_2} \qquad (4.6)$$

with

$$a = \omega^2,\ b = \omega^3,\ c_2 = \omega^2\Delta^2 - i\omega^3\Delta + i\omega\gamma'(2\Delta - i\omega) \text{ and } c_1 = \gamma'(2\Delta - i\omega) \qquad (4.7)$$

We notice that the function g(x) is odd and so we can transform the expression (4.5) to

$$\xi(-i\omega) = \frac{\beta}{2\pi} - \frac{\beta}{\pi i}\int_0^\infty g(x)f(x)dx + \frac{\beta}{2\pi i}\int_0^\infty g(x)dx \qquad (4.8)$$

where f(x) is the Fermi function. At absolute zero temperature the Fermi function vanishes and we only need to evaluate the last integral of Eq.(4.8). For small frequency range, $b^2 < 4ac_2$ and we can perform the integral quite easily giving

$$\int_0^\infty g(x)dx = \frac{4c_1}{\sqrt{4ac_2 - b^2}} \tan^{-1} \frac{b}{\sqrt{4ac_2 - b^2}} \qquad (4.9)$$

where

$$\frac{4c_1}{\sqrt{4ac_2 - b^2}} = \frac{4\gamma'(2\Delta - i\omega)}{\omega^{3/2}[4(\omega\Delta^2 - i\omega^2\Delta + \gamma'\omega + 2i\gamma'\Delta) - \omega^3]^{\frac{1}{2}}} \qquad (4.10)$$

and

$$\frac{b}{\sqrt{4ac_2 - b^2}} = \frac{\omega^{3/2}}{[4(\omega\Delta^2 - i\omega^2\Delta + \gamma'\omega + 2i\gamma'\Delta) - \omega^3]^{\frac{1}{2}}} \qquad (4.11)$$

We simplify the square of the last expression and obtain

$$\frac{b^2}{4ac_2 - b^2} = \frac{1}{\frac{4}{\tilde{\omega}^2} + \frac{4\delta}{\tilde{\omega}^2} + \frac{8i\delta}{\tilde{\omega}^3} - \frac{4i}{\tilde{\omega}} - 1} \qquad (4.12)$$

where

$$\delta = \gamma'/\Delta^2 \quad \text{and} \quad \tilde{\omega} = \omega/\Delta$$

The next step is to assume $\omega << \gamma'^{\frac{1}{2}}$. This assumption restricts the validity of our calculations to frequencies

very much smaller than $\sim 10^{12}$Hz. Since, $\gamma' = \frac{N_i \Delta}{\pi \rho} \approx \frac{N_i T_k}{\rho}$

at T = 0 and with the density of conduction electron states near the Fermi surface for both spins, $\frac{3N}{2\varepsilon_F}$, $\gamma' \approx cT_k\varepsilon_F$

where $c = N_i/N$ is the concentration of impurities. Hence $\omega_{max} \sim c^{\frac{1}{2}}\sqrt{\varepsilon_F T_k}$ is 10^{12}Hz, if we take $\varepsilon_F \sim 5$ ev and $T_k \sim 10^{\circ}$K.

Now, if we take $\omega^2 << \gamma'$, $\delta = \frac{\gamma'}{\Delta} >> \tilde{\omega}^2$. Using this condition, one can show that the expression (4.12) is very much less than 1 and hence the expansion for $\tan^{-1}x$ for small x is valid. Then $\tilde{\omega}^2 << \delta$ i.e. $\delta/\tilde{\omega}^2 >> 1$ and we can neglect 1 in the denominator of (4.12) compared to $\delta/\tilde{\omega}^2$. We obtain

$$\frac{1}{\frac{4}{\tilde{\omega}^2} + \frac{4\delta}{\tilde{\omega}^2} + \frac{4i}{\tilde{\omega}}\left[\frac{2\delta}{\tilde{\omega}^2} - 1\right]} = \frac{1}{\frac{4}{\tilde{\omega}^2} + \frac{4\delta}{\tilde{\omega}^2} + \frac{8i\delta}{\tilde{\omega}^3}} = \frac{\tilde{\omega}^2/4}{1 + \delta + 2i\delta/\tilde{\omega}} \tag{4.13}$$

We can consider two cases, $\delta \geq 1$ and $\delta \leq 1$. For both the possible cases the expression (4.13) is very much less than 1. Thus Eq.(4.9) can be expressed as

$$\int_0^\infty g(x)dx = \frac{4\gamma'(2\Delta - i\omega)}{4\omega\Delta^2 + 4\gamma'\omega - \omega^3 + 8i\gamma'\Delta - 4i\omega^2\Delta}$$

The rearranging and the rationalising of the r.h.s. gives

$$\frac{8\Delta\gamma'\omega(4\Delta^2+\omega^2)}{\omega^2(4\Delta^2+4\gamma'-\omega^2)^2+16\Delta^2(2\gamma'-\omega^2)^2} + i\frac{4\gamma'[\omega^2(4\Delta^2-4\gamma'+\omega^2)-16\gamma'\Delta^2]}{\omega^2(4\Delta+4\gamma'-\omega^2)+16\Delta^2(2\gamma'-\omega^2)^2} \tag{4.14}$$

Using (4.14), Eq.(4.8) becomes, at absolute zero temperature,

$$\xi(-i\omega) = \beta\left\{\frac{1}{2\pi} - \frac{i}{2\pi}\,\frac{8\Delta\gamma'\omega(4\Delta^2+\omega^2)}{\omega^2(4\Delta^2+4\gamma'-\omega^2)^2+16\Delta^2(2\gamma'-\omega^2)^2}\right.$$

$$\left. + \frac{1}{2\pi}\,\frac{4\gamma[\omega^2(4\Delta^2-4\gamma'+\omega^2)-16\gamma'\Delta^2}{\omega^2(4\Delta^2+4\gamma'-\omega^2)^2+16\Delta^2(2\gamma'-\omega^2)^2}\right\} \qquad (4.15)$$

Substituting Eq.(4.15) in Eq. (4.1), and dividing by $i\omega A_\mu$, one obtains the expression for complex conductivity given by

$$\sigma(\omega) = -\frac{2\pi}{3}\,\frac{e^2}{m^{*2}v}\,\rho k_F^2\left\{\frac{-i}{2\pi\omega} - \frac{1}{2\pi}\,\frac{8\Delta\gamma'(4\Delta^2+\omega^2)}{\omega^2(4\Delta^2+4\gamma'-\omega^2)^2+16\Delta^2(2\gamma'-\omega^2)^2}\right.$$

$$\left. - \frac{i}{2\pi}\,\frac{4\gamma[\omega(4\Delta^2-4\gamma'+\omega^2)-16\gamma'\Delta^2/\omega]}{\omega^2(4\Delta^2+4\gamma'-\omega^2)^2+16\Delta^2(2\gamma'-\omega^2)^2}\right\} \qquad (4.16)$$

The d.c. conductivity at T = 0 was found to be $\frac{1}{3}\,\frac{e^2}{m^{*2}v}\,\rho k_F^2\,\frac{\Delta}{2\gamma'} \equiv \sigma_o$. We can now express the real and imaginary parts of the frequency dependent conductivity in the dimensionaless form in the following manner

$$\tilde{\sigma}_R(\omega,0) = \frac{1+\frac{1}{4}\tilde{\omega}^2}{\left[1-\frac{1}{2}\,\frac{\tilde{\omega}^2}{\delta}\right]^2+\frac{1}{4}\tilde{\omega}^2\left[1+\frac{1}{\delta}-\frac{1}{4}\,\frac{\tilde{\omega}^2}{\delta}\right]^2} \qquad (4.17)$$

and

$$\tilde{\sigma}_I(\omega,0) = \frac{\tilde{\omega}\{[\frac{1}{\delta}+\frac{1}{2}\frac{\tilde{\omega}^2}{\delta}]-[1+\frac{1}{4}\tilde{\omega}^2]+\frac{1}{16}\,\frac{\tilde{\omega}^4}{\delta}\}}{2\left[1-\frac{1}{2}\,\frac{\tilde{\omega}^2}{\delta}\right]^2+\frac{\tilde{\omega}^2}{2}\left[1+\frac{1}{\delta}-\frac{1}{4}\,\frac{\tilde{\omega}^2}{\delta}\right]^2} \qquad (4.18)$$

where

$$\tilde{\sigma}_R(\omega,0) = \sigma_R(\omega,0)/\sigma_o \text{ and } \tilde{\sigma}_I(\omega,0) = \sigma_1(\omega,0)/\sigma_o$$

Now, $\delta = \frac{\gamma'}{\Delta^2} \sim c(\varepsilon_F/T_k)$ measures the impurity concentration. Also we assumed $\omega^2 << \gamma'$ which implies $\tilde{\omega}^2 << \delta$ i.e. $\frac{\tilde{\omega}^2}{\delta} << 1$. Using this limit Eqs.(4.17) and (4.18) reduce to

$$\tilde{\sigma}_R(\omega,0) = \frac{1 + \frac{1}{4}\tilde{\omega}^2}{1 + \frac{1}{4}\tilde{\omega}^2[1 + \frac{1}{\delta}]^2} \tag{4.19}$$

$$\tilde{\sigma}_I(\omega,0) = \frac{\frac{\tilde{\omega}}{2\delta}[1-\delta-\frac{1}{4}\delta\tilde{\omega}^2]}{1 + \frac{1}{4}\tilde{\omega}^2[1 + \frac{1}{\delta}]^2} \tag{4.20}$$

Before considering the pure and dirty limits i.e. $\delta << 1$ and $\delta >> 1$ we shall take into account the effect of temperature being increased from zero degree.

4.3 The A.C. Conductivity in the Pure and Dirty Limits

As temperature rises from the zero degree we cannot ignore the first integral of Eq.(4.8). We see that in the integral $\int_o^\infty f(x)g(x)dx$ the important values of x are of the order T_k and an expansion in powers of x is valid. So, we write

$$g(x) = \frac{c_1}{ax^2 - bx + c_2} - \frac{c_1}{ax^2 + bx + c_2}$$

$$\cong \frac{2bc_1}{c_2^2}x\left\{1 - \frac{2ac_2-b^2}{c_2^2}x^2 - \frac{a^2}{c_2^2}x^4 + \left(\frac{2ac_2-b^2}{c_2^2}\right)^2 x^4 + \ldots\right\}$$

$$\equiv d_1x + d_2x^3 + d_3x^5 + \ldots\ldots \text{ etc.} \tag{4.21}$$

with

$$d_1 = \frac{2bc_1}{c_2^2} \qquad d_2 = -\frac{2bc_1}{c_2^4}(2ac_2 - b^2) \text{ etc.} \tag{4.22}$$

We have assumed, $[(2ac_2 - b^2)/C_2^2]^{\frac{1}{2}} < 1$. In the limiting case this gives $\tau\sqrt{\frac{a}{c_2}} \sim 1$, i.e. $T \sim \gamma'^{\frac{1}{2}}$. Now, since $\Delta << \gamma'^{\frac{1}{2}}$, and for maximum frequency $\omega \sim 10^{12}$Hz, we get $T \sim 50$ K°if we take $\omega \sim \Delta$. Hence, our expansion is valid as long as the temperature is below 50°K. Since our expression for the average current is valid for temperatures below T_k, we are within our region of interest.

Now we write the integral in the following way

$$\sum_{r=1}^{\infty}(-1)^{r+1}\int_0^{\infty} g(x)e^{-r\beta x}dx = \sum_{r=1}^{\infty}(-1)^{r+1}\left[\int_0^{\infty} d_1 x e^{-\beta r x}dx + \int_0^{\infty} d_2 x^3 e^{-\beta r x}dx + \ldots\right] \tag{4.23}$$

and since

$$\int_0^{\infty} xe^{-rx}dx = \frac{1}{(\beta r)^2}, \quad \int_0^{\infty} x^3 e^{-\beta r x}dx = \frac{6}{(\beta r)^4}$$

also

$$\sum_{r=1}^{\infty}(-1)^{r+1}\frac{1}{r^2} = \frac{\pi^2}{12}, \quad \sum_{r=1}^{\infty}(-1)^{r+1}\frac{1}{r^4} = \frac{7}{720}x^4$$

Eq. (4.23) gives

$$\frac{d_1}{\beta^2}\frac{\pi^2}{12} + \frac{d_2}{\beta^4}\frac{7}{720}\pi^4 + \ldots . \tag{4.24}$$

Since the parameter (T/Δ) is very much less than unity, we can ignore all higher order contributions. Using definitions of a_1 b_1 c_1 and c_2 we get d_1, given by

$$\frac{2bc_1}{c_2^2} = \frac{4\omega\gamma'\Delta - 2i\omega^2\gamma'}{[\omega\Delta^2 - i\omega^2\Delta + 2i\gamma'\Delta + \gamma'\omega]^2} .$$

Rationalising, the above expression becomes

$$\frac{2bc_1}{c_2^2} = \frac{4\omega\gamma'\Delta[\omega^2(\Delta^2+\gamma')^2-\Delta^2(2\gamma'-\omega^2)^2]-4\omega^3\Delta\gamma'(\Delta^2+\gamma')(2\gamma'-\omega^2)}{[\omega^2(\Delta^2+\gamma')^2-\Delta^2(2\gamma'-\omega^2)^2]^2+4\Delta^2\omega^2(\Delta^2+\gamma')^2(2\gamma'-\omega^2)^2}$$

$$-i\frac{2\omega^2\gamma'[\omega^2(\Delta^2+\gamma')^2-\Delta^2(2\gamma'-\omega^2)^2]-8\omega^2\Delta^2\gamma'(\Delta^2+\gamma')(2\gamma'-\omega^2)}{[\omega^2(\Delta^2+\gamma')^2-\Delta^2(2\gamma'-\omega^2)^2]^2+4\Delta^2\omega^2(\Delta^2+\gamma')^2(2\gamma'-\omega^2)^2} \qquad (4.25)$$

This equation is substituted in Eq.(4.24), where we keep only the first term, and express it in dimensionless form as before. Then the real and imaginary parts of the complex conductivity can be written,using the same condition as before, as:

$$\tilde{\sigma}_R(\omega,T) = \frac{(1+\frac{1}{4}\tilde{\omega}^2)}{1+\frac{1}{4}\tilde{\omega}^2(1+\frac{1}{\delta})^2} + \frac{\pi^2}{3}\frac{4(1+\frac{\tilde{\omega}}{2})-\tilde{\omega}^2(1+\frac{1}{\delta})^2}{4[1+\frac{\tilde{\omega}^2}{2}(1+\frac{1}{\delta})^2+\frac{\tilde{\omega}^4}{16}(1+\frac{1}{\delta})^4]}(\frac{T}{\Delta})^2 \qquad (4.26)$$

$$\tilde{\sigma}_I(\omega,T) = \frac{\tilde{\omega}(\frac{1}{\delta}-1-\frac{1}{4}\tilde{\omega}^2)}{2[1+\frac{1}{4}\tilde{\omega}^2(1+\frac{1}{\delta})^2]} + \frac{\pi^2}{3}\frac{\tilde{\omega}[(1+\frac{2}{\delta})+\frac{\tilde{\omega}^2}{4}(1+\frac{1}{\delta})^2]}{2[1+\frac{\tilde{\omega}^2}{2}(1+\frac{1}{\delta})^2+\frac{\tilde{\omega}^4}{16}(1+\frac{1}{\delta})^4]}(\frac{T}{\Delta})^2 \qquad (4.27)$$

One can easily verify that for d.c. conductivity $\tilde{\sigma}_R(0,T) = [1 + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2]$ and $\tilde{\sigma}_I(0,T) = 0$ which is, of course, what it should be.

We now consider the two limiting cases:

1. In the pure limit, i.e. $\delta << 1$, for very low concentration of impurities, $\frac{1}{\delta} >> 1$ and we also have $\tilde{\omega}^2 << 1$ the Eqs.(4.26) and (4.27) reduce to

$$\tilde{\sigma}_R(\omega,T) = \frac{1}{1 + x^2} + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2 \frac{1 - x}{(1 + x^2)^2} \qquad (x = \tilde{\omega}/2\delta) \qquad (4.28)$$

$$\tilde{\sigma}_I(\omega,T) = \frac{x}{1 + x^2} + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2 \frac{\frac{1}{2}x}{(1 + x^2)^2} \qquad (4.29)$$

2. In the dirty limit, $\delta >> 1$, $\frac{1}{\delta} << 1$. We have to remember that our solutions are not valid for a very dirty limit, since the single particle Green's function we derived is valid only for low concentration of impurities. In this case, the Eqs. reduce to

$$\tilde{\sigma}_R(\omega,T) = 1 + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2 \frac{1}{1 + x^2} \qquad (x = \tilde{\omega}/2) \qquad (4.30)$$

$$\tilde{\sigma}_I(\omega,T) = - x + \frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2 \frac{x}{1 + x^2} \qquad (4.31)$$

Eqs. (4.30) and (4.31) are independent of impurity concentration.

4.4 Discussion

As mentioned earlier, in the absence of experimental data in the region of interest, we cannot compare our theory

with experimental results. In the dirty limit, our expression for complex conductivity becomes independent of impurity concentration. This has to be viewed with scepticism, since our solutions for the self-consistent equations are not valid for high concentration of impurities. In the pure limit, our expression for complex conductivity is given by a universal function of $\tilde{\omega}/\delta$. Murata and Wilkins[91] calculated numerically the surface resistance of Kondo alloys for several impurity concentrations. Our results seem to agree well with their predictions as far as variation with concentration of impurities is concerned. Theoretical calculations of Moriya and Inoue[90] as well as Murata and Wilkins[91] indicate that a peak might be observed in measurements of the surface impedance of a Kondo alloy at low temperatures in the microwave or far infrared spectral regions. The experimental results of Brändli[92] et al. do not show any peak. Although they argue that the presence of potential scattering will reduce the peaking behaviour, one can by no means be certain that the differential calculation of the A.C. response would show no peak experimentally. Our results do not show any peak although we have not taken potential scattering into account. But, unfortunately, we cannot claim our results to be valid in the far infrared frequency region because of the approximation involved. We believe that the so-called peak in the surface impedance measurements of Kondo alloys is yet to be established.

CHAPTER 5 EXTENDED INTERACTION FORMULATION

5.1 Introduction

In chapters 2 and 3 we have re-derived Nagaoka's equations in the presence of a uniform electromagnetic field, $\underset{\sim}{E}(t)$, and solved them by iteration procedure. We found that the vertex part does not contribute to the electrical conductivity of the system. In this section, we want to generalize Nagaoka's treatment to the case of an extended exchange interaction and see the effect of applying linear response to it. This time, because of the mathematical complexity, we formulate the equations, in the absence of the electromagnetic field, and the vertex corrections are taken into account through the Ward's Identity.

5.2 Formulation of the Equations

The Hamiltonian is written as

$$H = H_o + \sum_{\alpha} H_{ex}^{\alpha} \tag{5.1}$$

with

$$H_{ex}^{\alpha} = -\frac{1}{2N} \sum_{kk'} J_{kk'} e^{i(\underline{k}'-\underline{k})\cdot\underline{R}\alpha} \Big[(C_{k\uparrow}^{+} C_{k'\uparrow} - C_{k\downarrow}^{+} C_{k'\downarrow}) S_z^{\alpha}$$

$$+ C_{k\uparrow}^{+} C_{k'\downarrow} S_{-}^{\alpha} + C_{k\downarrow}^{+} C_{k'\uparrow} S_{+}^{\alpha} \Big] \tag{5.2}$$

H_o is the conduction electron energy as defined by Eq.(2.2). All quantities are defined in Sec.2.2. The only difference now is that in Eq.(5.1), J, the strength of

the exchange integral, now depends on the conduction electron momenta k and k', whereas in Eq.(2.1) it is a constant. We shall assume later that $J_{kk'}$ depends only on $|\underset{\sim}{k} - \underset{\sim}{k}'|$.

Now, we define the single particle Green's functions $G_{kk'}$, $\Gamma^{\alpha}_{kk'}$, and their boundary conditions, as before, (Sec. 2.2), and use the same decoupling procedure to arrive at the following set of Equations.

$$(i\omega_n - \varepsilon_{k'})G_{kk'}(\omega_n) + \frac{1}{2N}\sum_{\ell,\alpha} J_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha}_{k\ell}(\omega_n) = \frac{i}{\beta}\delta_{kk'} \tag{5.3}$$

$$\begin{aligned}
&[i\Omega(\omega_n) - \varepsilon_{k'}]\,\Gamma^{\alpha}_{kk'}(\omega_n) \\
&\quad + \tfrac{3}{4}\frac{1}{2N}\sum_{\ell} J_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}(\omega_n) \\
&\quad - \frac{1}{2N}\sum_{\ell} J_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha}_{k\ell}(\omega_n) \\
&\quad + \frac{1}{N}\sum_{\ell\ell'} J_{\ell\ell'} n^{\alpha}_{k'\ell} e^{i(\underline{\ell}'-\underline{k}').\underline{R}\alpha}\Gamma^{\alpha}_{k\ell'}(\omega_n) \\
&\quad - \frac{1}{2N}\sum_{\ell\ell'} J_{\ell\ell'} m^{\alpha}_{k'\ell} e^{i(\underline{\ell}'-\underline{k}').\underline{R}\alpha} G_{k\ell'}(\omega_n) = 0
\end{aligned} \tag{5.4}$$

Where $n^{\alpha}_{k'k}$ and $m^{\alpha}_{k'k}$ are

$$n^{\alpha}_{k'k} = e^{i(\underline{k}'-\underline{k}).\underline{R}\alpha} < C^{+}_{k\uparrow} C_{k'\uparrow} >$$

$$m^{\alpha}_{k'k} = 3e^{i(\underline{k}'-\underline{k}).\underline{R}\alpha} < C^{+}_{k\uparrow} C_{k'\downarrow} S^{\alpha}_{-} >$$

In the limit of low concentration of impurities ($c << 1$) we can replace $n^{\alpha}_{k'k}$ and $m^{\alpha}_{k'k}$ by their impurity averaged values,

$n_{k'k}$ and $m_{k'k}$, as we did before. Let us put

$$V_{k'k} = \sum_p J_{pk} n_{k'p} - \tfrac{1}{2} J_{k'k} \tag{5.5}$$

$$\Lambda_{k'k} = \sum_p J_{pk} m_{k'p} - \tfrac{3}{4} J_{k'k} \tag{5.6}$$

Then the Eqs. (5.3) and (5.4) reduce to

$$(i\omega_n - \varepsilon_{k'}) G_{kk'}(\omega_n) + \frac{1}{2N} \sum_{\ell,\alpha} J_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma^{\alpha}_{k\ell}(\omega_n) = \frac{i}{\beta}\delta_{kk'} \tag{5.7}$$

and

$$[i\Omega(\omega_n) - \varepsilon_{k'}]\Gamma^{\alpha}_{kk'}(\omega_n)$$

$$+ \frac{1}{N} \sum_{\ell} V_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma^{\alpha}_{k\ell}(\omega_n)$$

$$- \frac{1}{2N} \sum_{\ell} \Lambda_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}(\omega_n) = 0 \tag{5.8}$$

$n_{k'k}$ and $m_{k'k}$ are related to $G_{kk'}(\omega_n)$ and $\Gamma^{\alpha}_{kk'}(\omega_n)$ by the following relations

$$n_{k'k} = -i\, e^{i(\underline{k}'-\underline{k}).\underline{R}\alpha} \sum_{\omega_n} G_{kk'}(\omega_n) e^{i\omega_n 0+} \tag{5.9}$$

$$m_{k'k} = -2i\, e^{i(\underline{k}'-\underline{k}).\underline{R}\alpha} \sum_{\omega_n} \Gamma^{\alpha}_{kk'}(\omega_n) e^{i\omega_n 0+} \tag{5.10}$$

So Eqs. (5.7) to (5.10) together with Eqs. (5.5) and (5.6) now form a closed set of equations. We shall solve them for s and p wave scattering only.

5.3 Formal Solution with s and p Wave Scattering Only.

In the lowest order approximation we replace $[i\Omega(\omega_n) - \varepsilon_{k'}]$, appearing in Eq.(5.8), by $(i\omega_n - \varepsilon_{k'})$, and write Eqs. (5.7) and (5.8) in the following form

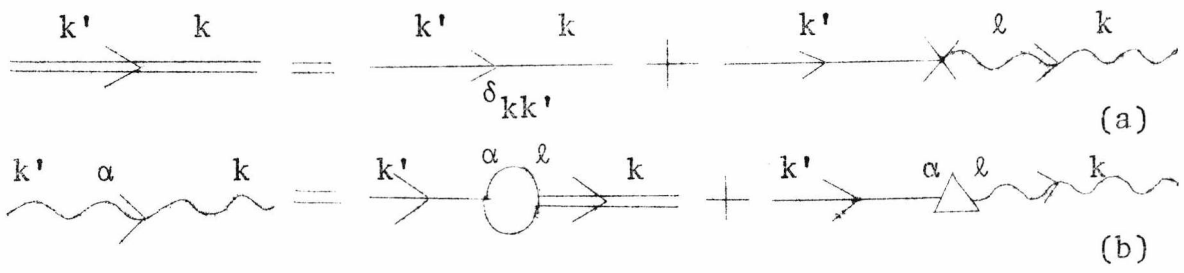
$$G_{kk'}(\omega_n) = g_k(i\omega_n)\delta_{kk'} + \frac{i\beta}{2N} g_{k'}(i\omega_n) \sum_{\ell,\alpha} J_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma^{\alpha}_{k\ell}(\omega_n) \tag{5.11}$$

$$\Gamma^{\alpha}_{kk'}(\omega_n) = -\frac{i\beta}{2N} g_{k'}(i\omega_n) \sum_{\ell} \Lambda_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} G_{k\ell}(\omega_n)$$

$$+ \frac{i\beta}{N} g_{k'}(i\omega_n) \sum_{\ell} V_{k'\ell} e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha} \Gamma^{\alpha}_{k\ell}(\omega_n) \tag{5.12}$$

where the free electron propagator $g_k(i\omega_n)$ is as defined by Eq.(3.13). We represent Eqs.(5.11) and (5.12) diagrammatically (Figure 10).

One must notice here that at cross vertex (x) the impurities are summed over, whereas at circle (O) and triangle (Δ) vertices they are not. $\Gamma^{\alpha}_{kk'}$ depends explicitly on the position of a single impurity at $\underset{\sim}{R}\alpha$. Now, we double iterate the equations diagrammatically and examine the different order terms in the series for $G_{kk'}(\omega_n)$. This series up to sixth order term, would be as shown in Figure 11.



where

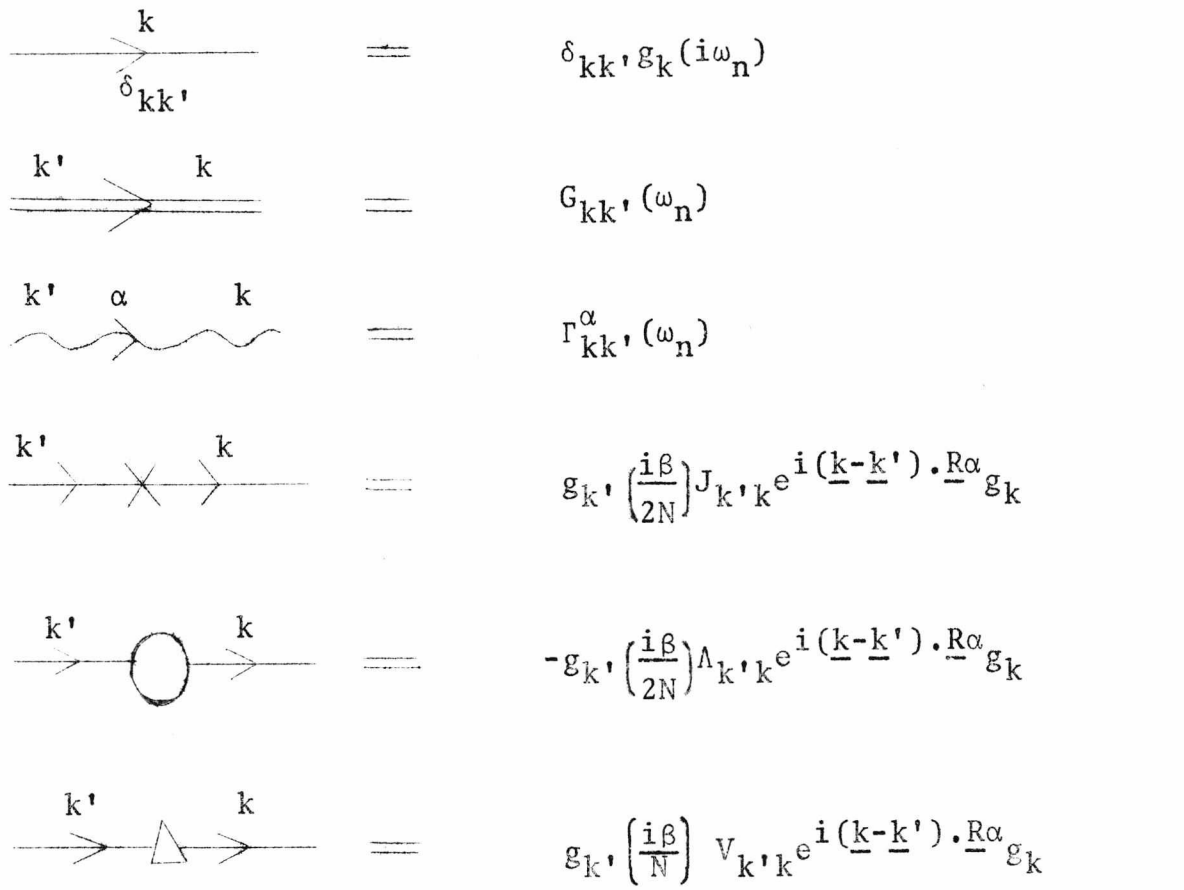


Figure 10 : Diagrammatic representation of Equations (5.11) and (5.12).

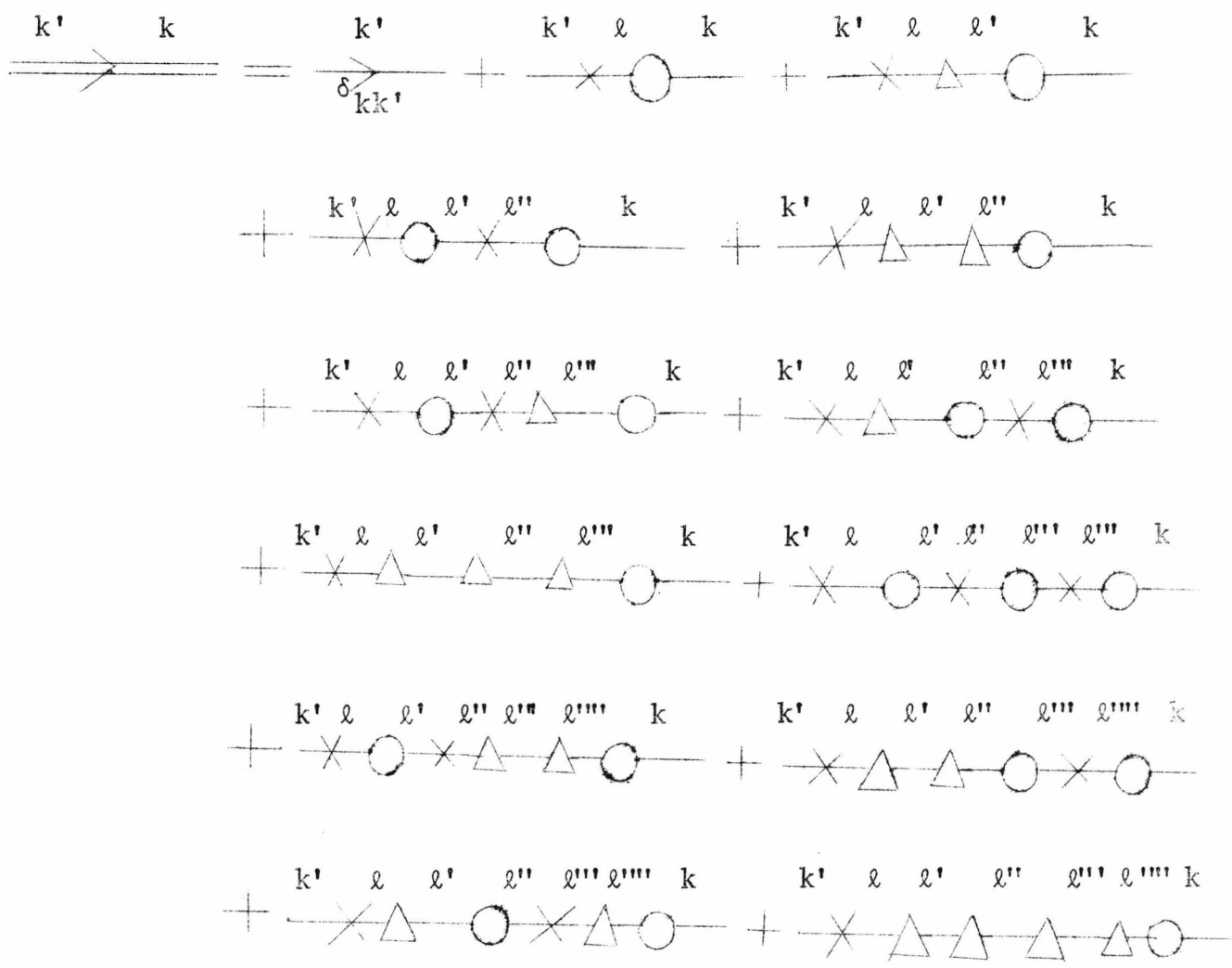


Figure 11 : Expansion of $G_{kk'}(\omega_n)$ up to sixth order.

A careful examination of the terms of various orders will reveal the pattern of the n^{th} order term. We find that the n^{th} order term, (i) starts with a cross and ends with an open circle; (ii) open circles and crosses occur in pairs, (iii) any number of triangles occur between the cross and open circle of (i). This pattern can be seen mathematically if we write the following matrix equations for G and Γ for (a) and (b) in Figure 10.

$$G = g + gX\Gamma$$

$$\Gamma = gOG + g\Delta\Gamma$$

Solving for G, one obtains

$$G = [1 - gX(1 - g\Delta)^{-1}gO]^{-1}g$$

Expanding, we can write

$$G = [1 - (gXgO + gXg\Delta gO + gXg\Delta g\Delta gO + \ldots)]^{-1}g$$

Suppressing g's, this series can be written as

$$\begin{aligned} G = {} & 1 + XO + X\Delta O + [XOXO + X\Delta\Delta O] \\ & + [XOXO + X\Delta OXO + X\Delta\Delta\Delta O] \\ & + [XOXOXO + XOX\Delta\Delta O + X\Delta\Delta OXO \\ & + X\Delta OX\Delta O + X\Delta\Delta\Delta\Delta O] + \ldots . \end{aligned} \qquad (5.13)$$

The general pattern of the terms occurring in the series for G can now be clearly perceived. Having been able to find the pattern, our next problem is to sum the series for G. The whole series for G can be diagrammatically written as shown in Figure 12.

Let us denote the series in Fig. 12 (d) by $\hat{G}_\alpha$, as it depends on the impurity position at $\underset{\sim}{R}\alpha$. Using the definitions (given in Fig. 10) we can write

$$\hat{G}_\alpha(k,k') = g_k\delta_{kk'} + \left(\frac{i\beta}{N}\right)g_{k'}\sum_{\ell}V_{k'\ell}e^{i(\underline{\ell}-\underline{k}').\underline{R}\alpha}\hat{G}_\alpha(k,\ell) \qquad (5.14)$$

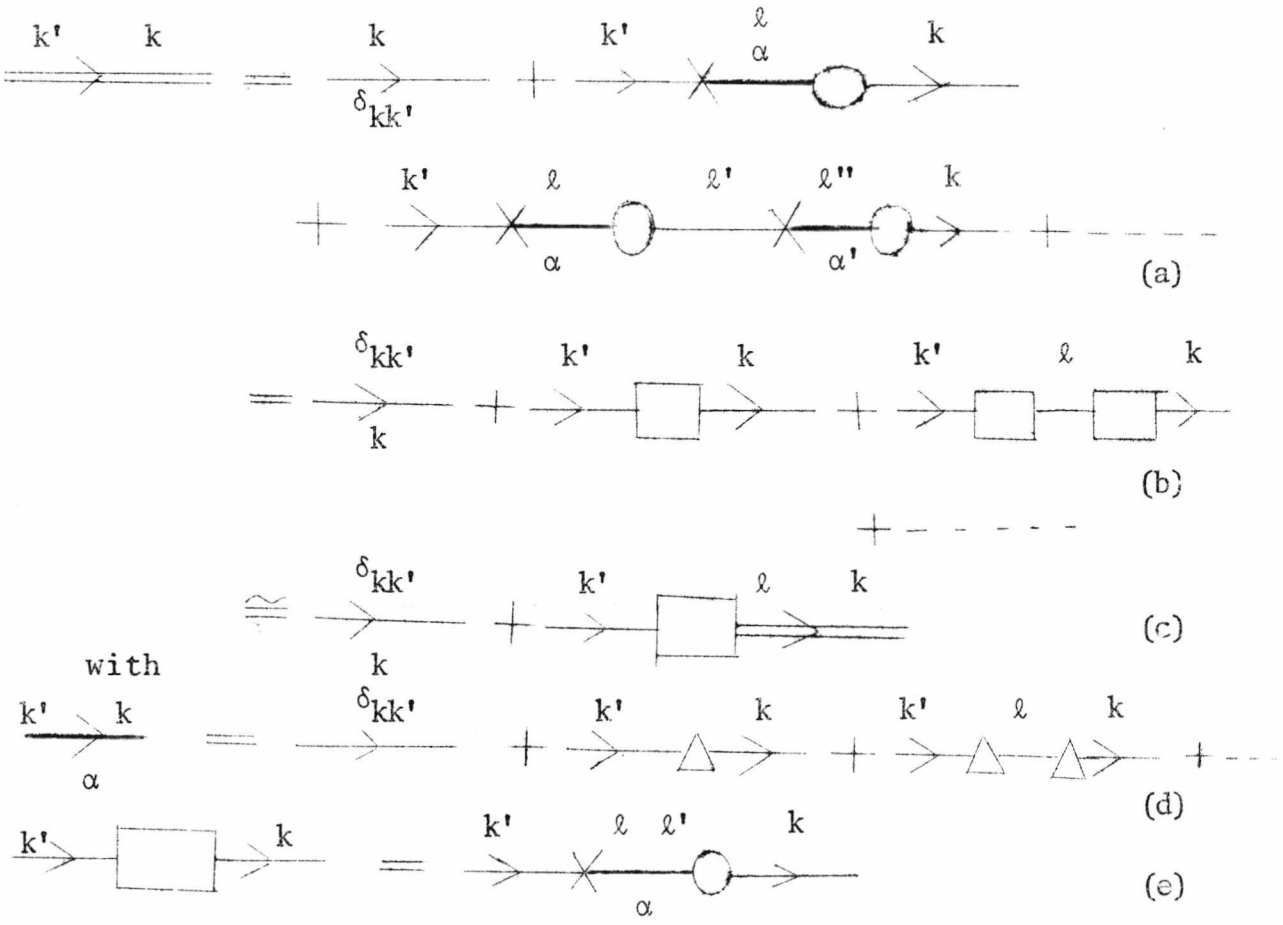


Figure 12 : The Series For $G_{kk'}$.

Let us try a solution of the form

$$\hat{G}_{\alpha}(k.k') = \hat{G}(k.k')e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} \tag{5.15}$$

Then Eq.(5.14) reduces to

$$\hat{G}(k,k') = g_k\delta_{kk'} + g_{k'}\left(\frac{i\beta}{N}\right)\sum_{\ell}V_{k'\ell}\hat{G}(k,\ell) \tag{5.16}$$

Hence Eq.(5.15) is indeed a solution of Eq.(5.14). Using Eq.(5.15), Fig. 12(e) can be written as

$$-g_{k'}\left(\frac{i\beta}{2N}\right)^2\sum_{\ell,\ell';\alpha}J_{k'\ell}\Lambda_{\ell'k}\hat{G}(\ell',\ell)e^{i(\underline{k}-\underline{k}').\underline{R}\alpha}g_k \tag{5.17}$$

and the series for $G_{kk'}(\omega_n)$, Fig. 12(c) is given by

$$G_{kk'}(\omega_n) = \delta_{kk'}g_k - g_{k'}\left(\frac{i\beta}{2N}\right)^2 \sum_{\ell,\ell'\alpha} J_{k'\ell}\Lambda_{\ell'k}\hat{G}(\ell',\ell)G_{k'\ell}(\omega_n)e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} \tag{5.18}$$

Then Eqs.(5.16) and (5.18) form two coupled equations for $\hat{G}(k,k')$ and $G_{kk'}(\omega_n)$. We have to solve them.

We now recall the approximation made in Eq.(5.12) where we replaced the renormalised propagator by a free electron propagator. This means that the interactions between the impurity spins at different sites have been neglected. And this is a good approximation in the limit of low concentration of impurities. But this simplification, later on, gives rise to divergent integrals in the vertex equations. We shall use the renormalised propagator to take into account the spin-spin interactions and replace it by the free electron propagator when it does not bring in any unnecessary mathematical complexity. Next, we must remember that if we sum the series for $G_{kk'}(\omega_n)$ by iteration, repeated scattering at a single site would give rise to 'nested diagrams'. Taking these into account, Eq.(5.16) is replaced by

$$\hat{G}(k,k') = G_k\delta_{kk'} + \left(\frac{i\beta}{N}\right)G_{k'}\sum_{\ell}V_{k'\ell}\hat{G}(k,\ell) \tag{5.19}$$

Now, these coupled Eqs. (5.18) and (5.19) are either impossible or extremely difficult to solve for the general case. We shall solve them for s and p wave scattering only.

The scattering of conduction electrons by a single impurity at $\underset{\sim}{R}\alpha$ depends only on $|\underline{k}-\underline{k}'|$ i.e. on the modulus of the difference of wave vectors of incoming and scattered waves. In the limit of low concentration of impurities, we can expand the exchange interaction, $J_{kk'}$ into Legendre polynomials, $P_\ell(\cos\theta_{kk'})$. We write

$$J_{kk'} = \sum_{\ell=o}^{\infty} (2\ell+1) J_\ell^{\ell}(\cos\theta_{kk'}) \quad .$$

For s and p wave scattering only this can be written as

$$J_{kk'} = J_o + J_1 \cos\theta_{kk'} \tag{5.20}$$

where J_o and J_1 are constants denoting the strengths of s and p wave scattering. Now, from the definitions of $V_{k'k}$ and $\Lambda_{k'k}$ given in Eqs. (5.5) and (5.6) and also from the solutions in Chapter 3 for s wave only, we can make the following ansätz:

$$V_{k'k} = V_{(o)}(k') + V_{(1)}(k')\cos\theta_{k'k} \tag{5.21}$$

$$\Lambda_{k'k} = \Lambda_{(o)}(k') + \Lambda_{(1)}(k')\cos\theta_{k'k} \tag{5.22}$$

Let us also assume a solution for $\hat{G}(k,k')$ of Eq.(5.19) given by

$$\hat{G}(k,k') = \delta_{kk'} G_k + \hat{G}_{(o)}(k,k') + \hat{G}_{(1)}(k,k')\cos\theta_{kk'} \tag{5.23}$$

where $\hat{G}_{(o)}(k,k')$ and $\hat{G}_{(1)}(k,k')$ depend on the modulii of k and k' only. Then substituting Eqs. (5.23) and (5.20) in Eq. (5.19) and equating the coefficients of $\cos\theta_{kk'}$ and unity

on both sides, one obtains

$$\hat{G}_{(o)}(k,k') = \frac{i\beta}{N} G_{k'} \{ V_{(o)}(k') G_k + V_{(o)}(k') \sum_{\ell} \hat{G}_{(o)}(k,\ell) \} \tag{5.24}$$

$$\hat{G}_{(1)}(k,k') = \frac{i\beta}{N} G_{k'} \{ V_{(1)}(k') G_k + \frac{1}{3} V_{(1)}(k') \sum_{\ell} \hat{G}_{(1)}(k,\ell) \} \tag{5.25}$$

Where some of the terms vanished due to angular integrations and use has been made of the following result,

$$\sum_{\ell} \cos\theta_{k\ell} \cos\theta_{\ell k'} = \frac{1}{3} \cos\theta_{kk'}$$

Solving for $\hat{G}_{(o)}(k,k')$ and $\hat{G}_{(1)}(k,k')$ in Eqs.(5.24) and (5.25), one gets

$$\hat{G}_{(o)}(k,k') = \left(\frac{i\beta}{N}\right) V_{(o)}(k') G_k G_{k'} \left[1 - i\beta \xi_{V_{(o)}} \right]^{-1} \tag{5.26}$$

and

$$\hat{G}_{(1)}(k,k') = \left(\frac{i\beta}{N}\right) V_{(1)}(k') G_k G_{k'} \left[1 - \frac{1}{3} i\beta \xi_{V_{(1)}} \right]^{-1} \tag{5.27}$$

where

$$\xi_{V_{(o)}} = \frac{1}{N} \sum_{k} V_{(o)}(k) G_k \tag{5.28}$$

$$\xi_{V_{(1)}} = \frac{1}{N} \sum_{k} V_{(1)}(k) G_k \tag{5.29}$$

Therefore, $\hat{G}(k,k')$ has a solution of the form

$$\hat{G}(k,k') = \delta_{kk'} G_k + \left(\frac{i\beta}{N}\right) V_{(o)}(k') G_k G_{k'} \left[1 - i\beta \xi_{V_{(o)}} \right]^{-1}$$

$$+ \left(\frac{i\beta}{N}\right) V_{(1)}(k') G_k G_{k'} \left[1 - \frac{1}{3} i\beta \xi_{V_{(1)}} \right]^{-1} \cos\theta_{kk'} \tag{5.30}$$

We can now find the impurity averaged value of $G_{kk'}$ for s and p wave scattering only by a similar technique to that applied in Chapter 3. This is illustrated in Figure 13.

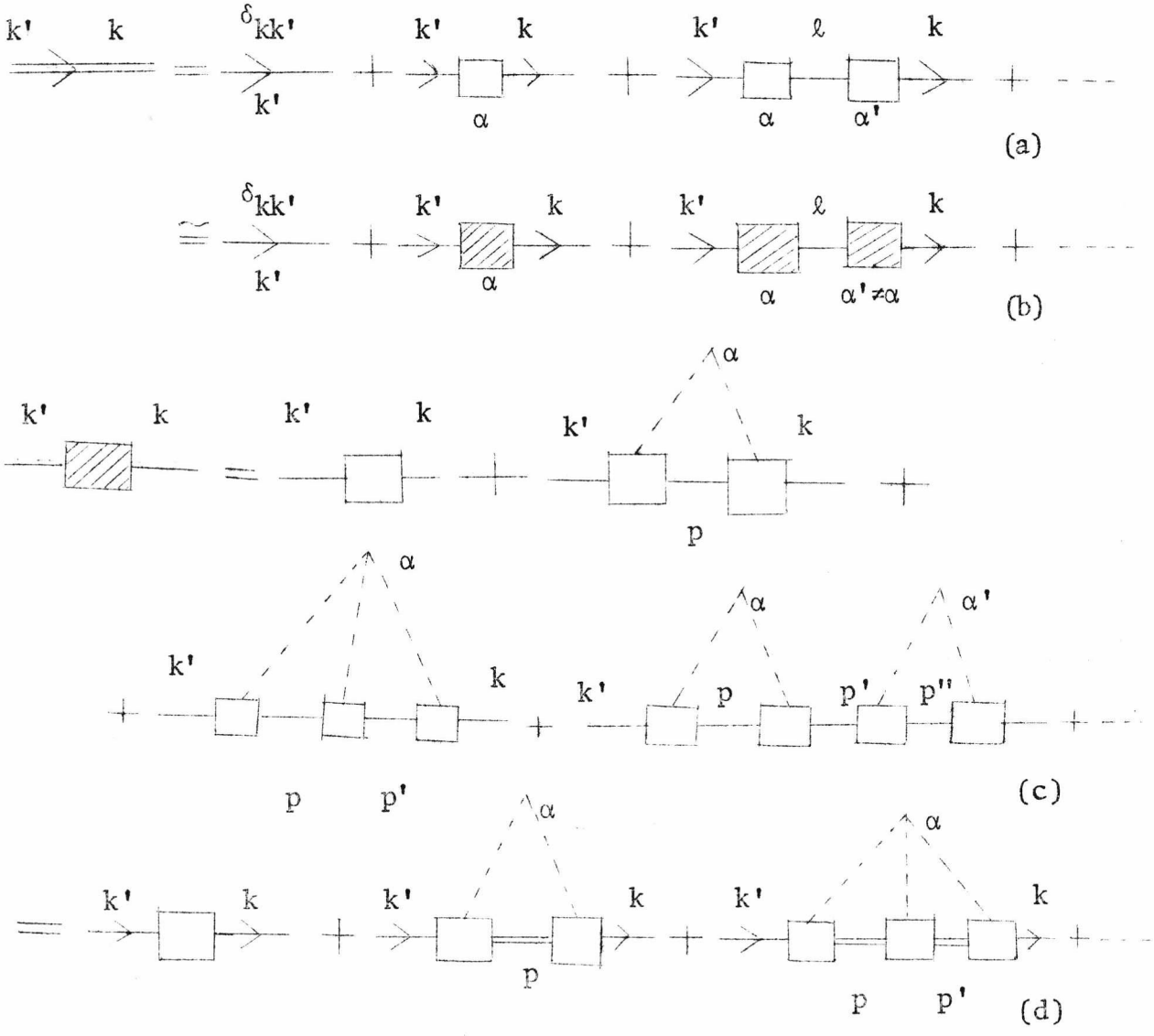


Figure 13 : Calculation of $G_{kk'}(\omega_n)$; (a) is the expansion of $G_{kk'}(\omega_n)$ and (b), (c) and (d) show an approximate calculation of it. Boxes connected with the dotted lines are associated with the same impurity.

The series in Fig. 13 (d) can be written as

$$-g_{k'}\left(\frac{i\beta}{2N}\right)^2 \sum_{\ell,\ell'} J_{k'\ell}\Lambda_{\ell'k}\hat{G}(\ell',\ell)e^{i(\underline{k}-\underline{k}')\cdot\underline{R}\alpha}g_k$$

$$+\left(\frac{i\beta}{2N}\right)^4 g_{k'}\sum_p \left\{\sum_{\ell,\ell'}[J_{k'\ell}\Lambda_{\ell'p}\hat{G}(\ell',\ell)]G_p \sum_{\ell'',\ell'''}[J_{p\ell''}\Lambda_{\ell'''k}\hat{G}(\ell''',\ell'')]\right\}$$

$$e^{i(\underline{k}-\underline{k}')\cdot\underline{R}\alpha}g_k$$

$$+ \ldots \qquad (5.31)$$

This series cannot be summed for the general case of all partial waves. We have succeeded in summing the series for s and p wave scattering only. Then, using Eqs. (5.20), (5.21) and (5.30), one obtains

$$\sum_{\ell,\ell'} J_{k'\ell}\Lambda_{\ell'k}\hat{G}(\ell',\ell) = \frac{NJ_o\eta_{(o)}}{1-i\beta\xi_{V_{(o)}}} + \frac{\frac{1}{3}J_1N\eta_{(1)}}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}}\cos\theta_{kk'} \qquad (5.32)$$

where

$$\eta_{(o)} = \frac{1}{N}\sum_k \Lambda_{(o)}(k)G_k \qquad (5.33)$$

$$\eta_{(1)} = \frac{1}{N}\sum_k \Lambda_{(1)}(k)G_k \qquad (5.34)$$

Similarly, one finds

$$\sum_{\ell,\ell'} J_{k'\ell}\Lambda_{\ell'p}\hat{G}(\ell',\ell) = \frac{NJ_o\eta_{(o)}}{1-i\beta\xi_{V_o}} + \frac{\frac{1}{3}J_1N\eta_{(1)}}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}}\cos\theta_{pk'} \qquad [5.34(i)]$$

and

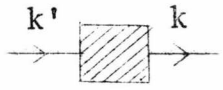
$$\sum_{\ell'',\ell'''} J_{p\ell''}\Lambda_{\ell'''k}\hat{G}(\ell''',\ell'') = \frac{NJ_o\eta_{(o)}}{1-i\beta\xi_{V_{(o)}}} + \frac{\frac{1}{3}J_1N\eta_{(1)}}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}}\cos\theta_{kp} \qquad [5.34(ii)]$$

and hence the term appearing in the curly bracket in the second term of Eq.(5.31) can be easily evaluated. One finds

$$\sum_p \left\{ \sum_{\ell,\ell'} [J_{k'\ell}\Lambda_{\ell'p}\hat{G}(\ell',\ell)] G_p \sum_{\ell'',\ell'''} J_{p\ell''}\Lambda_{\ell'''k}\hat{G}(\ell''',\ell'') \right\}$$

$$= \left\{ \left[\frac{J_o N\eta_{(o)}}{(1-i\beta\xi_{V_{(o)}})} \right]^2 + \frac{1}{3}\left[\frac{\frac{1}{3}J_1 N\eta_{(1)}}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}} \right]^2 \cos\theta_{kk'} \right\} \sum_p G_p \qquad (5.35)$$

One can see now that using Eqs.(5.32), (5.35) and other similar quantities, the series in Fig. 13 (d) can be written as

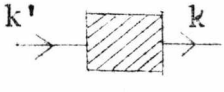


$$= -g_{k'}\left(\frac{i\beta}{2N}\right)^2 \left[\frac{NJ_o\eta_{(o)}}{1-i\beta\xi_{V_{(o)}}} + \frac{\frac{1}{3}J_1 N\eta_{(1)}}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}} \cos\theta_{kk'} \right] g_k e^{i(\underline{k}-\underline{k}').\underline{R}\alpha}$$

$$+ \left(\frac{i\beta}{2N}\right)^4 g_{k'} \sum_p G_p \left\{ \left[\frac{J_o N\eta_{(o)}}{1-i\beta\xi_{V_{(o)}}} \right]^2 + \frac{1}{3}\left[\frac{\frac{1}{3}J_1\eta_{(1)}^N}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}} \right]^2 \cos\theta_{kk'} \right\} g_k e^{i(\underline{k}-\underline{k}').\underline{R}\alpha}$$

$$+ \ldots\ldots .$$

We can sum this double geometric series to obtain



$$= -g_{k'}A_{(o)}e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} g_k - g_{k'}A_{(1)}\cos\theta_{kk'}e^{i(\underline{k}-\underline{k}').\underline{R}\alpha} g_k \qquad (5.36)$$

where $A_{(o)}$ and $A_{(1)}$ are

$$A_{(o)} = \frac{\left(\frac{i\beta}{2N}\right)^2 \frac{NJ_o\eta(o)}{1-i\beta\xi_{V_{(o)}}}}{\left[1 + \left(\frac{i\beta}{2N}\right)^2 \sum_p G_p \frac{J_o N\eta(o)}{1 - i\beta\xi_{V_{(o)}}}\right]} \tag{5.37}$$

$$A_{(1)} = \frac{\left(\frac{i\beta}{2N}\right)^2 \frac{\frac{1}{3}J_1 N\eta(1)}{1-\frac{1}{3}i\beta\xi_{V_{(1)}}}}{\left[1 + \frac{1}{3}\left(\frac{i\beta}{2N}\right)^2 \sum_p G_p \frac{\frac{1}{3}J_1\eta(1)^N}{1 - \frac{1}{3}i\beta\xi_{V_{(1)}}}\right]} \tag{5.38}$$

We now find the impurity averaged $\overline{G_{kk'}}(\omega_n)$ from Fig. 13(b) given by

$$\overline{G_{kk'}}(\omega_n) = \frac{g_k \delta_{kk'}}{[1 + N_i(A_{(o)}+A_{(1)})g_k]} \tag{5.39}$$

Eq.(5.39) can be written as

$$\overline{G_{kk}}(\omega_n) = \frac{i}{\beta} \frac{1}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \tag{5.40}$$

where, $\sum(\omega_n)$, the self-energy part, after some simplification, can be expressed as

$$\sum(\omega_n) = \frac{c}{4}\left\{\frac{\eta^o J_o}{1+\xi_o+\frac{1}{4}J_o\eta^o F} + \frac{\frac{1}{3}J_1\eta^1}{1+\frac{1}{3}\xi_1+\frac{1}{36}J_1\eta^1 F}\right\} \tag{5.41}$$

with c = Ni/N, the concentration of impurities and

$$\eta^{o} = \frac{1}{N} \sum_{k} \frac{\Lambda_{(o)}(k)}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \tag{5.42}$$

$$\eta^{1} = \frac{1}{N} \sum_{k} \frac{\Lambda_{(1)}(k)}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \tag{5.43}$$

$$\xi_{o} = \frac{1}{N} \sum_{k} \frac{V_{(o)}(k)}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \tag{5.44}$$

$$\xi_{1} = \frac{1}{N} \sum_{k} \frac{V_{(1)}(k)}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \tag{5.45}$$

and

$$F = \frac{1}{N} \sum_{k} \frac{1}{[i\omega_n - \varepsilon_k + \sum(\omega_n)]} \quad . \tag{5.46}$$

Thus, Eqs.(5.40) to (5.46) give formal solutions to our closed set of equations for the impurity averaged single-particle Green's function, where we have taken s and p wave scattering only. In the next chapter, we shall calculate the electrical conductivity of the Kondo system using this solution.

CHAPTER 6 SOLUTIONS : CONDUCTIVITIES AT HIGH AND LOW TEMPERATURES

6.1 Solution at High Temperatures

At high temperatures, $T > T_k$ we can apply perturbational treatment and so we put

$$m_{k'k} = 0 \quad \text{and} \quad n_{k'k} = f_k \delta_{kk'} \ . \tag{6.1}$$

Then, from definitions of $V_{(o)}(k)$, $V_{(1)}(k)$, $\Lambda_{(o)}(k)$ and $\Lambda_{(1)}(k)$ we have

$$\Lambda_{(o)}(k) = -\tfrac{3}{4} J_o \qquad V_o(k) = J_o(f_k - \tfrac{1}{2})$$

$$\Lambda_{(1)}(k) = -\tfrac{3}{4} J_1 \qquad V_{(1)}(k) = J_1(f_k - \tfrac{1}{2}) \tag{6.2}$$

Let us put,

$$i\omega_n + \sum(\omega_n) = i\Omega_n \tag{6.3}$$

and assume that Ω_n is real and has the same sign as ω_n. Both of these assumptions are consistent and we shall see that these assumptions do not lead to any contradiction. Then, we calculate the quantities F, η^o, η^1, ξ_o and ξ_1 as before (Chapter 3); we obtain

$$F = -i \frac{\pi\rho}{N} \operatorname{sign} \omega_n \tag{6.4}$$

$$\eta^o = i \tfrac{3}{4} \frac{\pi\rho}{N} J_o \operatorname{sign} \omega_n \tag{6.5}$$

$$\eta^1 = i \tfrac{3}{4} \frac{\pi\rho}{N} J_1 \text{sign } \omega_n \tag{6.6}$$

where ρ is the density of conduction electron states near the Fermi surface. We also have

$$\xi_o \cong \frac{\rho J_o}{2N} \int_{-D}^{D} \frac{\tanh(\frac{\epsilon}{2T})d\epsilon}{\epsilon - i\Omega_n} \tag{6.7}$$

At T = 0, this is

$$\xi_o = - \frac{\rho J_o}{N} \ell n|\frac{\Omega_n}{D}| \text{ for } D >> \Omega_n. \tag{6.8}$$

Again, we introduced the cut-off parameter D which is taken to be of the order of band-width. Similarly, at T = 0

$$\xi_1 = - \frac{\rho J_1}{N} \ell n|\frac{\Omega_n}{D}| \quad . \tag{6.9}$$

Since, at high temperatures, we are expanding the quantities in powers of J_o and J_1, we can ignore $\left(\frac{\rho J_o}{N}\right)^2$ and $\left(\frac{\rho J_1}{N}\right)^2$ compared to unity. Then $\sum(\omega_n)$ can be written as

$$\sum(\omega_n) = \frac{i\gamma_o \text{sign } \omega_n}{1-b_o \ell n|\frac{\Omega_n}{D}|} + \frac{i\gamma_1 \text{sign } \omega_n}{1-b_1 \ell n|\frac{\Omega_n}{D}|} \tag{6.10}$$

where

$$\gamma_o = \frac{3}{16} \frac{c\pi\rho}{N} J_o^2 \qquad \gamma_1 = \frac{1}{16} \frac{c\pi\rho}{N} J_1^2 \tag{6.11}$$

$$b_o = \frac{\rho J_o}{N} \qquad b_1 = \frac{1}{3} \frac{\rho J_1}{N} \tag{6.12}$$

It can be seen now by substituting Eq. (6.10) in Eq.(6.3) that the assumptions we made about Ω_n are consistent. We get

$$\Omega_n = \omega_n + \left[\frac{\gamma_o}{1-b_o \ell n \left|\frac{\Omega_n}{D}\right|} + \frac{\gamma_1}{1-b_1 \ell n \left|\frac{\Omega_n}{D}\right|} \right] \text{sign } \omega_n \qquad (6.13)$$

In the first order approximation, this is

$$\Omega_n = \omega_n + \left[\frac{\gamma_o}{1-b_o \ell n \left|\frac{\omega_n}{D}\right|} + \frac{\gamma_1}{1-b_1 \ell n \left|\frac{\omega_n}{D}\right|} \right] \text{sign } \omega_n \qquad (6.14)$$

$$\equiv \omega_n + f_o(\omega_n) \text{sign } \omega_n \, . \qquad (6.15)$$

where the function $f_o(\omega_n)$ is defined from the Eq.(6.14).

Next,we shall evaluate the average current and electrical conductivity of the system from the Kubo formula of linear response. We shall ignore the vertex corrections for the moment and later on take them into account. The current is given by

$$J_\mu = \beta v A_\nu \left(\frac{e}{m^* v}\right)^2 \sum_{k,\omega_n} k_\mu k_\nu \bar{G}_{kk}(\omega_n) \bar{G}_{kk}(\omega_n + \omega_p)$$

$$= -\frac{1}{3\beta} A_\mu \frac{e^2}{m^{*2} v} \rho k_F^2 \sum_{\omega_n} \int \frac{d\varepsilon}{[i\omega_n - \varepsilon + \sum(\omega_n)][i\omega_n + i\omega_p - \varepsilon + \sum(\omega_n + \omega_p)]} \qquad (6.16)$$

All the quantities are the same as defined in chapter 3. Performing the ε integral in the upper half plane, we

obtain

$$J_\mu = -\frac{1}{3\beta} A_\mu \frac{e^2}{m^{*2}v} \rho k_F^2 \sum_{-\omega_p<\omega_n<o} \frac{2\pi}{\omega_p + f_1(\omega_n) + f_2(\omega_n+\omega_p)} \tag{6.17}$$

where

$$f_1(\omega_n) = \frac{\gamma_o}{1-b_o \ell n \frac{\omega_n}{D}} + \frac{\gamma_1}{1-b_1 \ell n \frac{\omega_n}{D}} \tag{6.18}$$

and

$$f_2(\omega_n+\omega_p) = \frac{\gamma_o}{1-b_o \ell n \frac{\omega_n+\omega_p}{D}} + \frac{\gamma_1}{1-b_1 \ell n \frac{\omega_n+\omega_p}{D}} \tag{6.19}$$

We transform the ω_n-sum to a contour integral form as before, (See Chapter 3), and make analytic continuation to real frequencies $i\omega_p \to \omega + i0+$ to get

$$\sum_{-\omega_p<\omega_n<o} \frac{1}{\omega_p + f_1(\omega_n) + f_2(\omega_n + \omega_p)}$$

$$= \frac{\beta}{2\pi i} \int \frac{dx}{e^{\beta x}+1} [\phi(x) - \phi(x - \omega)] \tag{6.20}$$

with

$$\phi(x) = \frac{1}{-i\omega + \frac{\gamma_o}{1-b_o \ell n \frac{ix}{D}} + \frac{\gamma_o}{1-b_o \ell n \frac{-ix-i\omega}{D}} + \frac{\gamma_1}{1-b_1 \ell n \frac{ix}{D}} + \frac{\gamma_1}{1-b_1 \ell n \frac{-ix-i\omega}{D}}} \tag{6.21}$$

Using the same procedure the average current is found to be

$$J_\mu = iA_\mu \omega \frac{1}{3} \frac{e^2}{m^{*2}v} \rho k_F^2 \frac{1}{2(\gamma_o+\gamma_1)} \left\{ 1 - \frac{\gamma_o b_o + \gamma_1 b_1}{(\gamma_o+\gamma_1)} \ell n \left| \frac{T}{1.13D} \right| \right\} \tag{6.22}$$

and the conductivity is given by (in the d.c. limit)

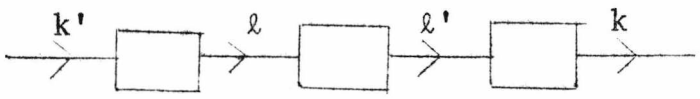
$$\sigma = \frac{ne^2}{m^*} \frac{8N}{3\pi\rho c(J_o^2+\frac{1}{3}J_1^2)} \left\{ 1 - \frac{\frac{\rho}{N}(J_o^3+\frac{1}{9}J_1^3)}{J_o^2+\frac{1}{3}J_1^2} \ell n \left| \frac{T}{1.13D} \right| \right\} \tag{6.23}$$

In the last expression we have replaced γ_o, γ_1, b_o and b_1 by their values from Eqs. (6.11) and (6.12). We notice that for $J_1 = 0$, i.e. for s-wave scattering only Eq.(6.23) immediately reduces to Eq.(3.55). The effect of taking p-wave scattering into account is just to renormalize the previous result for s-wave scattering only. But, we must also remember that we have not yet taken the vertex corrections into account. We shall do that in the following section.

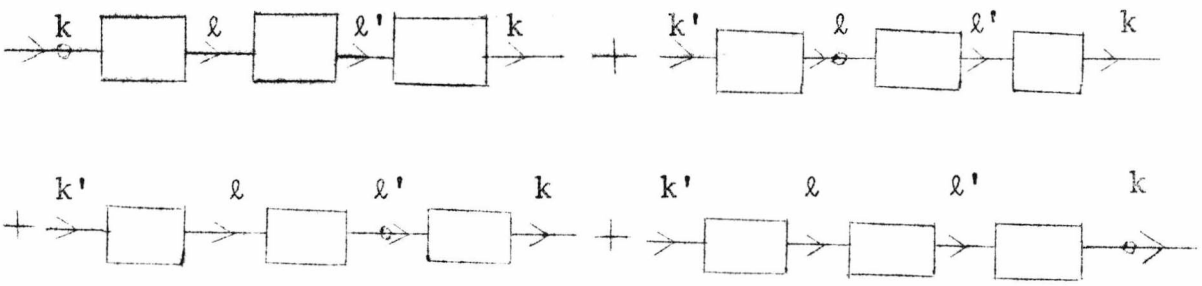
6.2 Vertex Corrections at High Temperatures

The vertex corrections are taken into account by the prescription laid down through the generalized Ward's identity which itself arises from the conservation laws, like the conservation of charge, particle, momentum etc. The series for the single particle Green's function is given by Fig.13(a) where the fundamental units are empty boxes. To take vertex corrections into account, one has to evaluate the vertex function which usually occurs in the form of an integral equation. According to the Ward's

identity, this integral equation has to be constructed by inserting current vertices at all points on the free electron propagator between the empty boxes, (in the diagram), in each term of the series. Only one current vertex has to be inserted at a time. At this point, we must recall that the empty boxes themselves consist of crosses, triangles and open circles, and notice that current vertices can also be inserted between them, but we shall consider this later. Thus, for the following typical term



we write



then the diagrams are bent about the vertices to form the vertex equation. Since, at high temperatures we expand in powers of J, we shall calculate the lowest order correction first. The vertex function, λ_μ is then given by the diagram 14 .

From Fig.14, the vertex equation is written as

$$\underset{\sim}{\lambda}_\mu(k) = \underset{\sim}{k}_\mu + \sum_{k',\alpha} \lambda_\mu(k')\bar{G}_{k'k'}(\omega_n)\bar{G}_{k'k'}(\omega_n + \omega_p)$$

$$\cdot\left(\frac{i\beta}{2N}\right)^4 \sum_{\ell,\ell'} J_{k\ell}\Lambda_{\ell'k'}\hat{G}(\ell',\ell,\omega_n)e^{i(\underline{k}'-\underline{k})\cdot\underline{R}\alpha}$$

$$\cdot \sum_{p,p'} J_{k'p}\Lambda_{p'k}\hat{G}(p',p,\omega_n+\omega_p)e^{i(\underline{k}-\underline{k}')\cdot\underline{R}\alpha} \qquad (6.24)$$

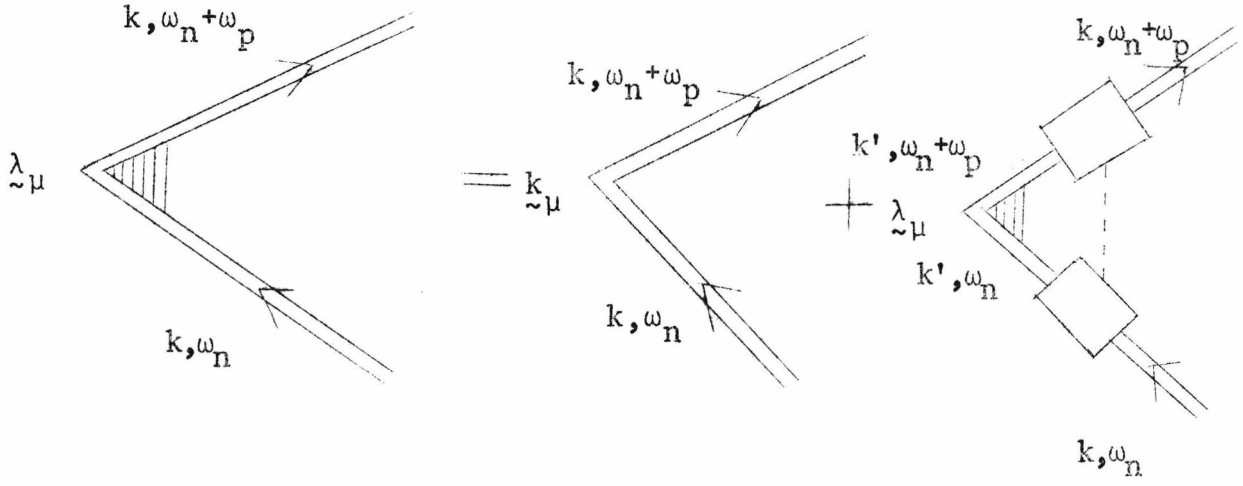


Figure 14 : The form of the integral equation for the vertex function, λ_μ.

As it is clear from the above Equation that the vertex function λ_μ does not depend on the position of a single impurity, the sum over the impurities can be performed immediately giving N_i, the total number of impurities in the system. We use Eqs. [5.34(i)] and [5.34(ii)] to reduce Eq. (6.24) in the following form

$$\underset{\sim}{\lambda}_\mu(k) = \underset{\sim}{k}_\mu + \left(\frac{i\beta}{2N}\right)^4 N_i(-i\beta N)^2 \sum_{k'} \Big\{ \underset{\sim}{\lambda}_\mu(k') G_{k'}(\omega_n) G_{k'}(\omega_n + \omega_p)$$

$$\cdot [J_o U_o(\omega_n) + J_1 U_1(\omega_n)\cos\theta_{kk'}]$$

$$\cdot [J_o U_o(\omega_n + \omega_p) + J_1 U_1(\omega_n + \omega_p)\cos\theta_{kk'}] \qquad (6.25)$$

where we wrote $\overline{G_{kk}} \equiv G_k$ and

$$U_o(\omega_n) = \frac{\eta^o(\omega_n)}{1 + \xi_o(\omega_n)} \quad \text{and} \quad U_1(\omega_n) = \frac{\frac{1}{3}\eta^1(\omega_n)}{1 + \frac{1}{3}\xi_1} \tag{6.26}$$

The Eq. (6.25) is very difficult to solve for the general case. Since λ_μ must be proportional to k_μ, we put $\underset{\sim}{\lambda}_\mu(k) = k_\mu \underset{\sim}{\lambda}(k)$ and multiply both sides by k_μ and sum over μ. The important k' values in the sum are $|\underset{\sim}{k}'| \sim k_F$ and also we require $\underset{\sim}{\lambda}(k)$ for $|\underset{\sim}{k}| \sim k_F$. Writing $\lambda(k_F) = \lambda$, we obtain

$$\lambda = 1 + \lambda \frac{(i\beta)^2}{16N^2} N_i \frac{1}{3} J_o J_1 \sum_{k'} \Big\{ [U_o(\omega_n)U_1(\omega_n+\omega_p) + U_1(\omega_n)U_o(\omega_n+\omega_p)] \cdot G_{k'}(\omega_n) G_{k'}(\omega_n + \omega_p) \Big\} \tag{6.27}$$

The product terms $U_o(\omega_n)U_o(\omega_n+\omega_p)$ and $U_1(\omega_n)U_1(\omega_n+\omega_p)$ vanished because of the angular integrations. Denoting

$$Q(\omega_n+\omega_p) = \int \frac{d\varepsilon}{[\varepsilon - i\omega_n - \sum(\omega_n)][\varepsilon - i\omega_n - i\omega_p - \sum(\omega_n+\omega_p)]} \tag{6.28}$$

Eq. (6.27) becomes

$$\lambda = \frac{1}{1 - \frac{N_i \rho}{48N^2} J_o J_1 \{Q(\omega_n+\omega_p)[U_o(\omega_n)U_1(\omega_n+\omega_p) + U_1(\omega_n)U_o(\omega_n+\omega_p)]\}} \tag{6.29}$$

Thus, in the simplest case the vertex function is given by

Eq. (6.29). Now, the conductivity is given by the current-current correlation function, represented by diagram 15, where the propagators are full Green's functions.

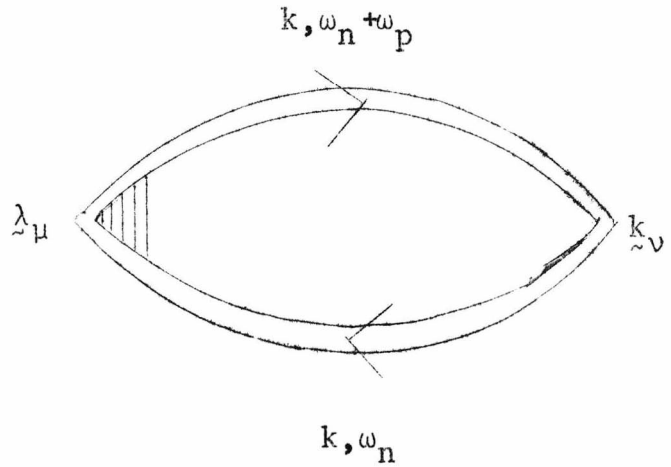


Figure 15 : The diagram representing the current-current correlation function.

The current is given by

$$J_\mu = \beta\nu\left(\frac{e}{m^*v}\right)^2 A_\nu \sum_{k,\omega_n} \lambda_\mu k_\nu G_k(\omega_n) G_k(\omega_n+\omega_p) \qquad (6.30)$$

All quantities appear in Eq. (6.30) are already defined in Chapter 3. Using Eq. (6.29) and performing the ε integrals in Eqs. (6.28) and (6.30), we obtain

$$j_\mu = -\frac{2\pi}{3\beta}\frac{e^2}{m^{*2}v} A_\mu k_F^2 \rho \sum_{-\omega_p<\omega_n<0} \Big\{ \omega_p + f_1(\omega_n) + f_2(\omega_n+\omega_p) - \alpha_o [U_o(\omega_n)U_1(\omega_n+\omega_p) + U_1(\omega_n)U_o(\omega_n+\omega_p)] \Big\}^{-1} \qquad (6.31)$$

where $f_1(\omega_n)$ and $f_2(\omega_n+\omega_p)$ are defined in Eqs. (6.18) and

(6.19) and we put $\alpha_o = \frac{c\rho}{48N} J_o J_1$. The ω_n sum is performed in the same way as before and we make analytic continuation, $i\omega_p \to \omega + i0+$ to get

$$j_\mu = -\frac{2\pi}{3\beta}\frac{e^2}{m^{*2}v} A_\mu k_F^2 \rho \frac{\beta}{2\pi i}\int \frac{dx}{e^{\beta x}+1}\left\{\phi(x) - \phi(x-\omega)\right\} \tag{6.32}$$

where

$$\phi(x) = \left\{-i\omega + \frac{\gamma_o}{1-b_o \ell n \frac{ix}{D}} + \frac{\gamma_o}{1-b_o \ell n \frac{-ix-i\omega}{D}} + \frac{\gamma_1}{1-b_1 \ell n \frac{ix}{D}} - \frac{\gamma'}{\left(1-b_o \ell n \frac{ix}{D}\right)\left(1-b_1 \ell n \frac{-ix-i\omega}{D}\right)} - \frac{\gamma'}{\left(1-b_o \ell n \frac{-ix-i\omega}{D}\right)\left(1-b_1 \ell n \frac{ix}{D}\right)}\right\}^{-1}$$

(6.33)

where b_o, b_1, γ_o and γ_1 are defined in Eqs. (6.11) and (6.12) and we put $\gamma' = \frac{c\pi^2\rho^3}{768N^3} J_o^2 J_1^2$. Expanding for $\frac{\rho J_o}{N} << 1$ and $\frac{\rho J_1}{N} << 1$, we get conductivity in the d.c. limit, given by

$$\sigma = \frac{1}{3}\frac{e^2}{m^{*2}v}\rho k_F^2 \frac{1}{2(\gamma_o+\gamma_1-\gamma')}\left[1 - \frac{\gamma_o b_o + \gamma_1 b_1 - 2\gamma' b_o b_1}{(\gamma_o+\gamma_1-\gamma')} \ell n \left|\frac{T}{1.13D}\right|\right]$$

$$= \frac{ne^2}{m^*}\frac{8N}{3\pi c\rho}\frac{1}{\left(J_o^2+\frac{1}{3}J_1^2 - \frac{\pi\rho^2}{144N^2}J_o^2J_1^2\right)}\left[1 - \frac{\frac{\rho}{N}\left(J_o^3+\frac{1}{9}J_1^3 - \frac{\pi\rho}{72N}J_o^3J_1^3\right)}{\left(J_o^2+\frac{1}{3}J_1^2 - \frac{\pi\rho^2}{144N^2}J_o^2J_1^2\right)} \ell n \left|\frac{T}{1.13D}\right|\right]$$

(6.34)

It is clear from Eq.(6.34) that the inclusion of vertex corrections by inserting current vertices between the empty boxes, contributes a correction which is sixth order in J, to the log term. In the high temperature expansion this is negligible.

To obtain the lower order correction, we need to write down the empty boxes in the series for the Green's function in their constituent crosses, triangles and open circles, and then apply the generalized Ward's identity as before. The Green's function is then given by

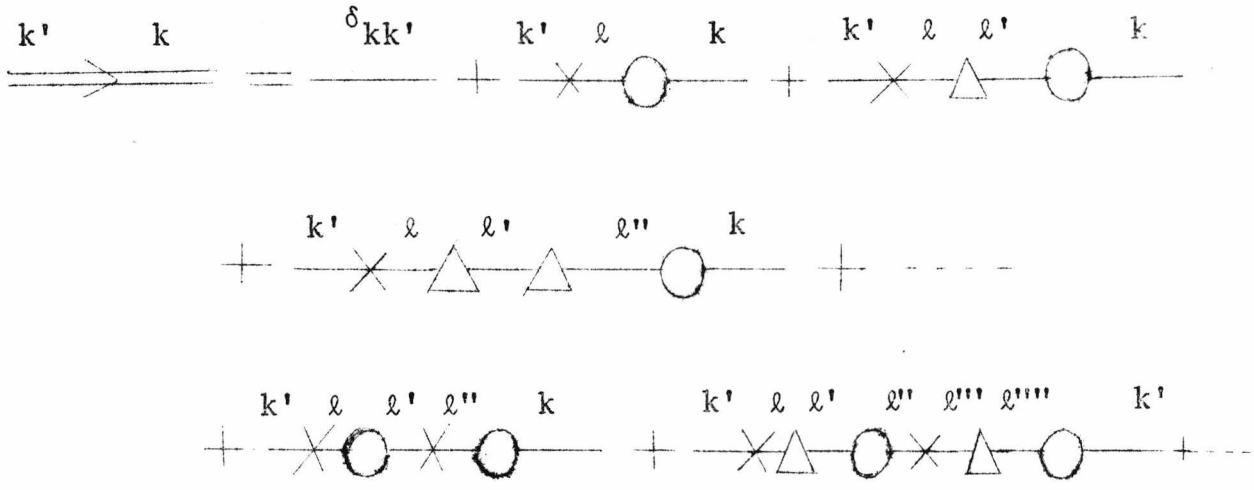


Figure 16 : The series for the Green's function $G_{kk'}$.

Inserting current vertices systematically and keeping only the first order corrections, the vertex equation can be represented as in Figure 17.

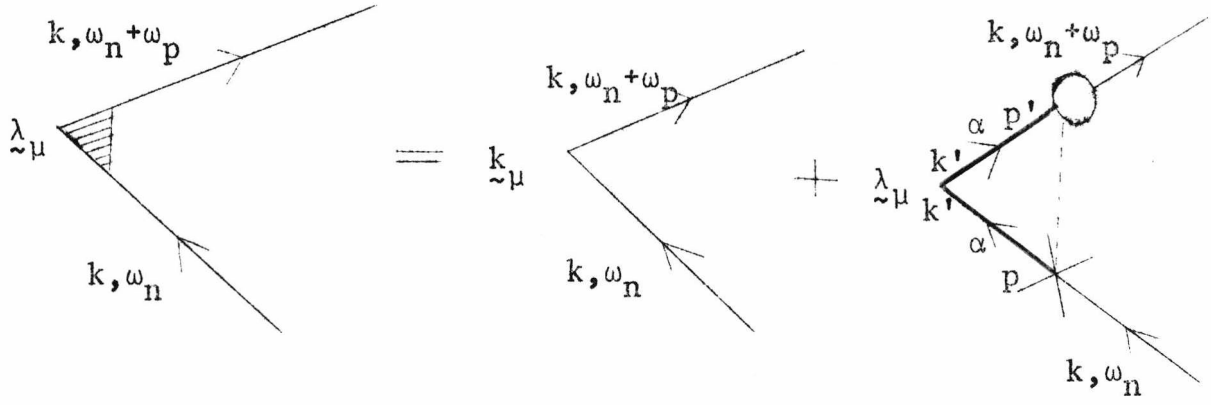


Figure 17 : The vertex equation for $\underset{\sim}{\lambda}_\mu$.

The open circle, cross and thick lines are all defined before in Chapter 5. The vertex equation is

$$\underset{\sim}{\lambda}_\mu(k) = \underset{\sim}{k}_\mu + \frac{\beta^2}{4N^2} \sum_{\substack{p,p' \\ k',\alpha}} \lambda_\mu(k')\hat{G}(k',p,\omega_n)\hat{G}(p',k',\omega_n+\omega_p)J_{kp}\Lambda_{p'k} \qquad (6.35)$$

Proceeding in the same way, writing $\lambda(k_F) \equiv \lambda$, one obtains

$$\lambda = \frac{1}{\left[1 - \frac{\beta^2 c}{4N} \sum_{\substack{p,p' \\ k'}} \mu\, \hat{G}(k',p,\omega_n)\hat{G}(p',k',\omega_n+\omega_p)J_{kp}\Lambda_{p'k}\right]} \qquad (6.36)$$

where, we put $\mu = \cos\theta_{kk'}$, which occurs when we multiply both sides of Eq.(6.35) by k_μ, sum over μ and divide both sides

by k^2. We shall now embark on calculating λ. This is a rather tedious job, but if we keep only terms third order in J, the algebra is simplified to a great extent. Now, using the values of $\hat{G}(k,k',\omega_n)$, $J_{kk'}$ and $\Lambda_{kk'}$ found for s and p wave scattering only, the term appearing in the denominator of the Eq. (6.36) can be written as

$$\sum_{\substack{p,p'\\k'}} \mu\hat{G}(k',p,\omega_n)\hat{G}(p',k',\omega_n+\omega_p)J_{kp}\Lambda_{p'k}$$

$$= -\frac{3}{4}\sum_{k',p'}\cos\theta_{kk'}(J_o+J_1\cos\theta_{kp})(J_o+J_1\cos\theta_{p'k})\Bigg\{\delta_{k'p}G_{k'}(\omega_n)$$

$$+\left(\frac{i\beta}{N}\right)V_{(o)}(p)G_pG_k\left[1-i\beta\xi_{V_{(o)}}(\omega_n)\right]^{-1}+\left(\frac{i\beta}{N}\right)V_{(1)}(p)G_{k'}(\omega_n)G_p(\omega_n)$$

$$\cdot\left[1-\frac{1}{3}i\xi_{V_{(1)}}(\omega_n)\right]^{-1}\cos\theta_{k'p}\Bigg\}$$

$$\cdot\Bigg\{\delta_{p'k'}G_{k'}(\omega_n+\omega_p)+\left(\frac{i\beta}{N}\right)G_{p'}(\omega_n+\omega_p)G_{k'}(\omega_n+\omega_p)V_{(o)}(k')[1-i\beta\xi_{V_{(o)}}(\omega_n+\omega_p)]^{-1}$$

$$+\left(\frac{i\beta}{N}\right)G_{p'}(\omega_n+\omega_p)G_{k'}(\omega_n+\omega_p)V_{(1)}(k')[1-\frac{1}{3}i\beta\xi_{V_{(1)}}(\omega_n+\omega_p)]^{-1}\cos\theta_{p'k'}\Bigg\}$$

(6.37)

At high temperatures, we put $m_{k'k} = 0$ and so $\Lambda_{k'k}$ becomes $-\frac{3}{4}J_{k'k}$. Now, we notice that the angular integrations will give zero for a large number of terms in Eq.(6.37). We perform the angular integrations and use Eq.(6.2) to obtain the following, keeping only terms up to third order in J,

$$\sum_{\substack{p,p'\\k'}} \mu \hat{G}(k',p,\omega_n)\hat{G}(p',k',\omega_n+\omega_p)J_{kp}\Lambda_{p'k}$$

$$= -\frac{J_o J_1}{4}\Bigg\{ 2\sum_{k'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)$$

$$+ \left(\frac{i\beta}{N}\right)J_o \sum_{k',p'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)G_{p'}(\omega_n+\omega_p)(f_{k'}-\tfrac{1}{2})$$

$$+ \left(\frac{i\beta}{N}\right)J_o \sum_{k',p'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)G_{p'}(\omega_n)(f_{p'}-\tfrac{1}{2})$$

$$+ \frac{1}{3}\left(\frac{i\beta}{N}\right) J_1 \sum_{k',p'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)G_{p'}(\omega_n)(f_{p'}-\tfrac{1}{2})$$

$$+ \frac{1}{3}\left(\frac{i\beta}{N}\right) J_1 \sum_{k',p'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)G_{p'}(\omega_n+\omega_p)(f_{k'}-\tfrac{1}{2})\Bigg\}$$

(6.38)

The k' and p' sums appearing in the above expression are independent of each other and can be performed separately without much difficulty. However, the sums with the factor $(f_{k'}-\frac{1}{2})$ or $(f_{p'}-\frac{1}{2})$ (f_k is the Fermi distribution function) are evaluated at T = 0. We obtain the following results

$$\text{(i)}\quad \sum_{k'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p) = -\frac{2\pi\rho}{\beta^2}\,\frac{1}{\omega_p + f_1(\omega_n) + f_2(\omega_n+\omega_p)}$$

$$= -\frac{2\pi\rho}{\beta^2}\,\frac{1}{Q(\omega_n+\omega_p)} \qquad (-\omega_p<\omega_n<o)$$

(6.39)

ρ is the density of states of conduction electrons near the Fermi surface and the functions $f_1(\omega_n)$ and $f_2(\omega_n+\omega_p)$ are already defined and $Q(\omega_n+\omega_p)$ is defined from its previous line.

$$\text{(ii)} \quad \sum_{p'} G_{p'}(\omega_n+\omega_p) \cong \frac{\pi\rho}{\beta}\text{sign}(\omega_n+\omega_p) = \frac{\pi\rho}{\beta} \text{ for } -\omega_p<\omega_n<o \qquad (6.40)$$

$$\text{(iii)} \quad \sum_{k'} G_{k'}(\omega_n)(f_{k'},-\tfrac{1}{2}) \cong -\frac{i\rho}{\beta}\ell n\left|\frac{\omega_n+f_1(\omega_n)}{D}\right| = -\frac{i\rho}{\beta}\ell n\left|\frac{A(\omega_n)}{D}\right| \qquad (6.41)$$

$$\text{(iv)} \quad \sum_{k'} G_{k'}(\omega_n)G_{k'}(\omega_n+\omega_p)(f_{k'}-\tfrac{1}{2})$$

$$\cong -\frac{i\rho}{\beta^2}\frac{1}{\omega_p+f_1(\omega_n)+f_2(\omega_n+\omega_p)}\ell n\left|\frac{\omega_n+f_1(\omega_n)}{\omega_n+\omega_p+f_2(\omega_n+\omega_p)}\right|$$

$$= -\frac{i\rho}{\beta^2}\frac{1}{Q(\omega_n+\omega_p)}\ell n\left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right| \qquad (6.42)$$

The functions $A(\omega_n)$ and $B(\omega_n+\omega_p)$ are defined quite obviously from the above expressions. Now using these results [Eqs. (6.39) to (6.42)] the expression (6.38) is simplified to the form

$$\frac{J_o J_1 \pi\rho}{\beta^2}\frac{1}{Q(\omega_n+\omega_p)}\left\{1-\frac{\rho}{4N}(J_o+\frac{1}{3}J_1)\ell n\left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right| + \frac{\rho}{2N}(J_o+\frac{1}{3}J_1)\ell n\left|\frac{A(\omega_n)}{D}\right|\right\} \qquad (6.43)$$

Substitution of Eq. (6.43) in Eq. (6.30) yields

$$\lambda = \frac{1}{\left\{1 - \frac{\alpha}{Q(\omega_n+\omega_p)} + \frac{\eta}{Q(\omega_n+\omega_p)} \ell n \left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right| - \frac{2\eta}{Q(\omega_n+\omega_p)} \ell n \left|\frac{A(\omega_n)}{D}\right|\right\}} \qquad (6.44)$$

where

$$\alpha = \frac{J_o J_1 \pi \rho N_i}{4N^2} = \frac{J_o J_1 \pi \rho c}{4N}$$

$$\eta = \frac{\rho}{4N} (J_o + \frac{1}{3} J_1)\alpha \quad .$$

6.3 Conductivity at High Temperatures

Now, the current is given, as usual, by

$$j_\mu = \beta v A_\nu \left(\frac{e}{m^* v}\right)^2 \sum_{k,\omega_n} k_\mu \lambda_\nu G_k(\omega_n) G_k(\omega_n+\omega_p)$$

Using the vertex function as obtained in Eq.(6.44), this becomes

$$j_\mu = -\frac{2\pi}{3\beta} \frac{e^2}{m^{*2} v} A_\mu k_F^2 \rho \sum_{-\omega_p < \omega_n < o} \frac{1}{\left\{Q(\omega_n+\omega_p) - \alpha + \eta \ell n \left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right| - 2\eta \ell n \left|\frac{A(\omega_n)}{D}\right|\right\}} \qquad (6.45)$$

The ω_n-sum is again performed by transforming it to a contour integral. After making analytic continuation as before, the ω_n sum becomes

$$\frac{\beta}{2\pi i} \int \frac{dx}{e^{\beta x}+1} [\phi(x) - \phi(x - \omega)] \qquad (6.46)$$

with

$$\phi(x) = \frac{1}{\left\{Q(-ix-i\omega)-\alpha+\eta\ell n\left[\frac{-A(-ix)}{B(-ix-i\omega)}\right]-2\eta\ell n\left[\frac{-A(-ix)}{D}\right]\right\}}$$

In the d.c. limit Eq. (6.46) is

$$-\frac{i\omega\beta}{2\pi}\int\phi(x)\Big|_{\omega=o}\left(-\frac{\partial f(x)}{\partial x}\right)dx \qquad (6.47)$$

Now, since

$$B(-ix-i\omega) = -ix-i\omega + \frac{\gamma_o}{1-b_o\ell n\frac{-ix-i\omega}{D}} + \frac{\gamma_1}{1-b_1\ell n\frac{-ix-i\omega}{D}}$$

$$A(-ix) = -ix - \frac{\gamma_o}{1-b_o\ell n\frac{ix}{D}} - \frac{\gamma_1}{1-b_1\ell n\frac{ix}{D}}$$

and

$$Q(-ix-i\omega) = B(-ix-i\omega) - A(-ix)$$

$$= -i\omega + \frac{\gamma_o}{1-b_o\ell n\frac{-ix-i\omega}{D}} + \frac{\gamma_1}{1-b_1\ell n\frac{-ix-i\omega}{D}} + \frac{\gamma_o}{1-b_o\ell n\frac{ix}{D}} + \frac{\gamma_1}{1-b_1\ell n\frac{ix}{D}}$$

On expansion, for $b_o\ell nT/D << 1$, $b_1\ell nT/D << 1$ and keeping terms only up to third order in J, one gets

$$\phi(x)\Big|_{\omega=o} \cong \frac{1}{2(\gamma_o+\gamma_1)-\alpha+[2(\gamma_o b_o+\gamma_1 b_1-\eta)\ell n\left|\frac{x}{D}\right|]}$$

Expanding once more

$$\phi(x)\Big|_{\omega=o} \cong \frac{1}{[2(\gamma_o+\gamma_1)-\alpha]}\left\{1 - \frac{2(\gamma_o b_o+\gamma_1 b_1-\eta)}{2(\gamma_o+\gamma_1)-\alpha}\,\ell n\left|\frac{x}{D}\right|\right\} \qquad (6.48)$$

Thus, the expression for current becomes

$$j_\mu = \frac{1}{3}\frac{e^2}{m^{*2}v}k_F^2\rho i\omega A_\mu \frac{1}{[2(\gamma_o+\gamma_1)-\alpha]}\left\{1 - \frac{2(\gamma_o b_o+\gamma_1 b_1-\eta)}{2(\gamma_o+\gamma_1)-\alpha}\,\ell n\left|\frac{T}{1.13D}\right|\right\} \qquad (6.49)$$

and the conductivity, σ is given by

$$\sigma = \frac{ne^2}{m^*}\,\frac{8N}{3\pi\rho c}\,\frac{1}{(J_o^2+\frac{1}{3}J_1^2-\frac{2}{3}J_oJ_1)}\left\{1 - \frac{\frac{\rho}{N}(J_o^3+\frac{1}{9}J_1^3-\frac{1}{3}J_o^2J_1-\frac{1}{9}J_1^2J_o)}{(J_o^2+\frac{1}{3}J_1^2-\frac{2}{3}J_oJ_1)}\,\ell n\left|\frac{T}{1.13D}\right|\right\} \qquad (6.50)$$

where we put back the values of b_o, b_1, γ_o, γ_1, η and α .

Now, we shall examine the implication of this expression for conductivity. We notice that if we put $J_1 = 0$ i.e. if we consider s-wave scattering only Eq.(6.50) immediately reduces to the Nagaoka expression, as it should be. We find that inclusion of vertex corrections gives rise to correction which is third order in J, and appears in the coefficient of the log term in the expression for conductivity. The denominator of the coefficient can be reduced to $(J_o - \frac{1}{3}J_1)^2 + \frac{2}{9}J_1^2$, which is always positive for any values of J_o and J_1. In the numerator, if we set $J_1 = rJ_o$, we get

$$\frac{\rho J_o^3}{9N}(r^3 - r^2 - 3r + 9).$$

And hence, when $r^3 - r^2 - 3r + 9 = 0$ the log term in the expression for conductivity vanishes, though we still have an interacting system. It is crucial to understand that the interference between s and p wave scattering can in fact 'wipe out' the logarithmic behaviour in the limiting case. The cubic equation for the ratio of J_1 and J_0 has one real root at~ -2.2. That is, at that particular ratio of J_1 and J_0, the leading logarithmic term vanishes though (as we shall show) the next order term does not. Hence, for particular dilute magnetic alloys with strong p wave scattering we obtain a different high temperature behaviour. It will be of interest to see how well these theoretical calculations agree with the experimental data. We shall discuss this point further in the last section of this chapter.

6.3(a) Calculating the next highest order term

Although it involves rather tedious algebra, we present here the calculation of the next highest order term and show that for the particular ratio of J_0 and J_1, when the leading logarithmic term vanishes, the next highest order term does not. The calculation is straightforward. From Eq. (6.37), we collect terms fourth order in J only and summations over momenta variables are carried out as before. The fourth order contribution to Eq. (6.43) is found to be

$$\frac{J_o J_1}{4}\Bigg\{-\frac{\pi\rho^3}{N^2\beta^2}\left(J_o^2+\frac{1}{9}J_1^2\right)\frac{1}{Q(\omega_n+\omega_p)}\ell n\left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right|\ell n\left|\frac{B(\omega_n+\omega_p)}{D}\right|$$

$$+\frac{2\pi\rho^3}{N^2\beta^2}\left(J_o^2+\frac{1}{9}J_1^2\right)\frac{1}{Q(\omega_n+\omega_p)}\ell n^2\left|\frac{A(\omega_n)}{D}\right|$$

$$-\frac{2\pi\rho^3}{3N^2\beta^2}J_o J_1\frac{1}{Q(\omega_n+\omega_p)}\ell n\left|\frac{A(\omega_n)}{B(\omega_n+\omega_p)}\right|\ell n\left|\frac{A(\omega_n)}{D}\right|\Bigg\} \qquad (6.51)$$

This is added to what we obtained before up to third order in J in Eq.(6.43). Following the same procedure, the expression for current becomes

$$j_\mu = -\frac{2\pi}{3\beta}\frac{e^2}{m^{*2}v}A_\mu k_F^2\rho\sum_{-\omega_p<\omega_n<o}\xi(\omega_n) \qquad (6.52)$$

with

$$\sum_{-\omega_p<\omega_n<o}\xi(\omega_n) = \frac{\beta}{2\pi i}\int\frac{dx}{e^{\beta x}+1}\Big\{\phi(x)-\phi(x-\omega)\Big\} \qquad (6.53)$$

and this time

$$\phi(x) = \Bigg\{Q(-ix-i\omega)-\alpha'+\alpha_1\ell n\left[\frac{A(-ix)}{B(-ix-i\omega)}\right]-2\alpha_1\ell n\left[\frac{-A(-ix)}{D}\right]+\alpha_2\ell n\left[\frac{B(-ix-i\omega)}{D}\right]$$

$$\cdot\,\ell n\left[\frac{-A(-ix)}{B(-ix-i\omega)}\right]-2\alpha_2\ell n^2\left[\frac{-A(-ix)}{D}\right]+\alpha_3\ell n\left[\frac{-A(-ix)}{B(-ix-i\omega)}\right]\ell n\left[\frac{-A(-ix)}{x}\right]\Bigg\}^{-1}$$

(6.54)

where

$$\alpha_1 = \frac{\pi c\rho^2}{16N^2} J_o J_1 (J_o + \frac{1}{3} J_1)$$

$$\alpha_2 = \frac{\pi\rho^3 c}{16N^3} J_o J_1 (J_o^2 + \frac{1}{9} J_1^2)$$

$$\alpha_3 = \frac{\rho^3 \pi c}{24N^3} J_o^2 J_1^2 \qquad (6.55)$$

and $$\alpha' = \frac{\pi\rho c}{4N} J_o J_1$$

All other quantities have been defined before. One has to be extremely cautious in including all fourth order terms. We recall the approximation made in $f_1(\omega_n)$ and $f_2(\omega_n+\omega_p)$, where we neglected higher order terms in J, because they are small compared to unity. We now keep these terms, and so the definitions of A(-ix) and B(-ix) are slightly modified. They are given by

$$A(-ix) = -ix + \frac{\gamma_o}{1-b_o \ell n \frac{ix}{D} + d_o} + \frac{\gamma_1}{1-b_1 \ell n \frac{ix}{D} + d_1} \qquad (6.56)$$

$$B(-ix) = -ix + \frac{\gamma_o}{1-b_o \ell n \frac{-ix}{D} + d_o} + \frac{\gamma_1}{1-b_1 \ell n \frac{-ix}{D} + d_1} \qquad (6.57)$$

where

$$d_o = \frac{3}{16} \frac{\pi^2\rho^2}{N^2} J_o^2 \quad \text{and} \quad d_1 = \frac{1}{48} \frac{\pi^2\rho^2}{N^2} J_1^2$$

Now, expanding, simplifying, and keeping only up to fourth

order terms in J, we get

$$\phi(x)\Big|_{\omega=o} \cong \frac{1}{[2(\gamma_o+\gamma_1)-\alpha']} \left\{1 - \frac{2(\gamma_o b_o + \gamma_1 b_1 - \alpha_1)}{[2(\gamma_o + \gamma_1) - \alpha']} \ell n\left|\frac{x}{D}\right| \right.$$

$$\left. - \frac{\pi^2(\alpha_2 - \frac{1}{2}\alpha_3) - \frac{\pi^2}{2}(\gamma_o b_o^2+\gamma_1 b_1^2) - 2(\gamma_o d_o+\gamma_1 d_1)}{[2(\gamma_o + \gamma_1) - \alpha']} - \frac{2(\gamma_o b_o^2+\gamma_1 b_1^2-\alpha_2)}{[2(\gamma_o+\gamma_1)-\alpha']} \ell n^2\left|\frac{x}{D}\right| \right\}$$

(6.58)

At this point, we may note that there is a constant fourth order term, (log independent), arising from the vertex equation we first formed by inserting current vertices between the empty boxes. Let us put that constant term together with that appearing in Eq. (6.58) to be equal to A_J,. We now insert Eq. (6.58) in Eq. (6.53) and label A_J to all constants arising there together with A_J,. We ignore this term because it is of no interest to us, since it can be easily verified that $1 - A_J > 0$, and therefore can be absorbed without difficulty. Finally, the conductivity is obtained as

$$\sigma \cong \frac{1}{3}\frac{e^2}{m^{*2}v} k_F^2 \rho \frac{1}{[2(\gamma_o+\gamma_1)-\alpha']} \left\{1 - \frac{2(\gamma_o b_o+\gamma_1 b_1-\alpha_1)}{[2(\gamma_o+\gamma_1)-\alpha']} \ell n\left|\frac{T}{1.13D}\right| \right.$$

$$\left. - \frac{2(\gamma_o b_o^2+\gamma_1 b_1^2-\alpha_2)}{[2(\gamma_o+\gamma_1)-\alpha']} \ell n^2 \frac{T}{D} \right\} \qquad (6.59)$$

We now examine the ℓn^2-term. The denominator of the coefficient is again always positive and the numerator can

be written as

$$\frac{\pi\rho^3 c}{8N^3}\left[3J_o^4 + \frac{1}{9}J_1^4 - J_o^3 J_1 - \frac{1}{9}J_o J_1^3\right]$$

Setting $J_1 = rJ_o$, this becomes

$$\frac{\pi\rho^3 c}{8N^3} J_o^4(r^4 - r^3 - 9r + 27)$$

and hence the particular value of the ratio $r(\simeq -2.2)$ for which the leading logarithmic term vanishes, the ℓn^2-term does not. But, since this is one order higher in J, its effect will be smaller. Hence, the gradual diminishing of logarithmic behaviour in certain alloys may be explained by taking the existence of strong p-wave scattering into account.

6.4 Conductivity at Low Temperatures

Our main interest has been to find out the effect of p-wave scattering on the electrical conductivity of the system and hence while solving the equations at low temperatures, we shall follow the easier method of Nagaoka. We assume

$$\Lambda_{(o)}(k) = \frac{\alpha^{(o)}}{\varepsilon_k} V_{(o)}(k) \qquad (6.60)$$

$$\Lambda_{(1)}(k) = \frac{\alpha^{(1)}}{\varepsilon_k} V_{(1)}(k) \qquad (6.61)$$

where $\alpha^{(o)}$ and $\alpha^{(1)}$ are parameters to be determined

self-consistently. Then, by substituting Eq. (6.60) in Eq. (5.42) we have

$$\frac{i\Omega_n}{\alpha^{(o)}}\eta^o = \xi_o + \frac{1}{N}\sum_k \frac{V_{(o)}(k)}{\varepsilon_k} \tag{6.62}$$

where we wrote, $i\omega_n + \sum(\omega_n) = i\Omega_n$ and similarly

$$\frac{i\Omega_n}{\alpha^{(1)}}\eta^1 = \xi_1 + \frac{1}{N}\sum_k \frac{V_{(1)}(k)}{\varepsilon_k} \tag{6.63}$$

Substitution of Eqs. (6.62) and (6.63) in Eq. (5.41) yields

$$\sum(\omega_n) = \frac{c}{4}\left\{\frac{J_o}{\frac{i\Omega_n}{\alpha^{(o)}} + \frac{1}{4}J_o F} + \frac{\frac{1}{3}J_1}{\frac{1}{3}\frac{i\Omega_n}{\alpha^{(1)}} + \frac{1}{36}J_1 F}\right\} \tag{6.64}$$

provided

$$1 - \frac{1}{N}\sum_k \frac{V_{(o)}(k)}{\varepsilon_k} = 0 \tag{6.65}$$

$$1 - \frac{1}{3N}\sum_k \frac{V_{(1)}(k)}{\varepsilon_k} = 0 \tag{6.66}$$

The last two equations determine $\alpha^{(o)}$ and $\alpha^{(1)}$. For $J_o < 0$ and $J_1 < 0$, we simplify $\sum(\omega_n)$ to obtain

$$\sum(\omega_n) = \frac{i\gamma_o \operatorname{sign}\Omega_n}{[|\Omega_n| + \Delta_{(o)}]} + \frac{i\gamma_1 \operatorname{sign}\Omega_n}{[|\Omega_n| + \Delta_{(1)}]} \tag{6.67}$$

$$\equiv if(\Omega_n)\operatorname{sign}\Omega_n \tag{6.68}$$

where we used Eq. (6.4) and replaced J_o, J_1 by their modulii and denoted

$$\gamma_o = c\, J_o\, \alpha^{(o)}/4 \qquad \gamma_1 = c\, J_1\, \alpha^{(1)}/4 \tag{6.69}$$

$$\Delta_{(o)} = \frac{\pi\rho\alpha^{(o)}}{4N} J_o \qquad \Delta_{(1)} = \frac{\pi\rho\alpha^{(1)}}{12N} J_1 \tag{6.70}$$

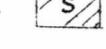
6.4(a) Self-consistent relations of $\Delta_{(o)}$ and $\Delta_{(1)}$

Before proceeding any further, we shall discuss the temperature dependence of $\Delta_{(o)}$ and $\Delta_{(1)}$. These quantities will be determined from Eqs. (6.65) and (6.66) and they in turn will fix $\alpha^{(o)}$ and $\alpha^{(1)}$. We recall the relations of $n_{kk'}$ and $m_{kk'}$ with $G_{k'k}$ and $\Gamma^{\alpha}_{k'k}$.

$$n_{kk'} = -i \sum_{\omega_n} e^{i(\underline{k}-\underline{k}')\cdot\underline{R}\alpha} G_{k'k}(\omega_n) e^{i\omega_n 0+} \equiv -i \sum_{\omega_n} \tilde{G}_{k'k} e^{i\omega_n 0+} \tag{6.71}$$

$$m_{kk'} = -2i \sum_{\omega_n} e^{i(\underline{k}-\underline{k}')\cdot\underline{R}\alpha} \Gamma^{\alpha}_{kk'}(\omega_n) e^{i\omega_n 0+} \equiv -2i \sum_{\omega_n} \tilde{\Gamma}_{k'k} e^{i\omega_n 0+} \tag{6.72}$$

We shall now evaluate $\tilde{G}_{k'k}$. This is slightly more complicated than the case we encountered before. The calculation is illustrated in Figure 18.

The difficulty arises because the momentum index k' is not summed over and we needed to construct a special impurity averaged box  . This special box is evaluated

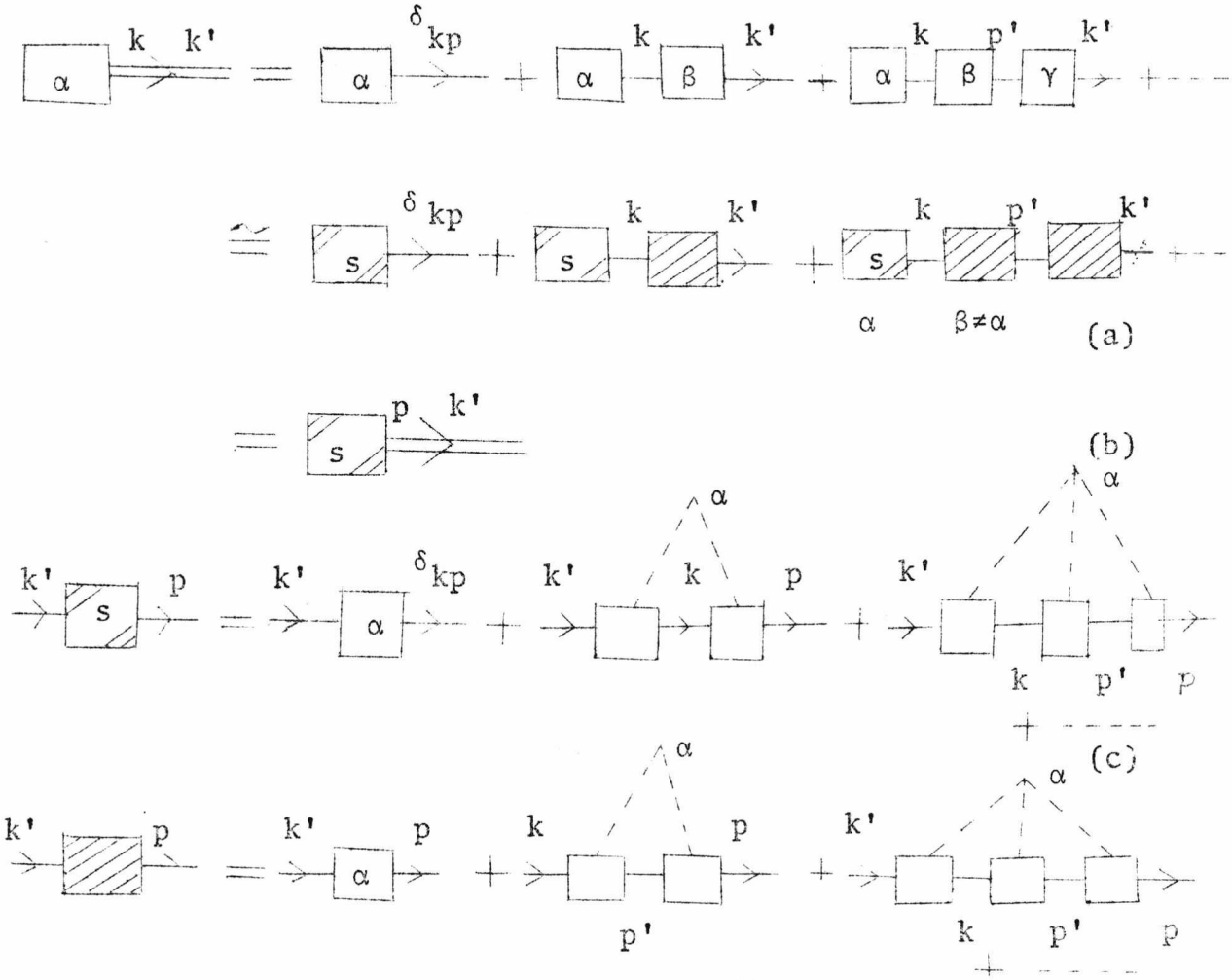


Figure 18 : Evaluation of $\tilde{G}_{k'k}$

in Fig. 18(c) and is found to be

$$\underset{(k)}{\boxed{s}} = U_{kk'}\delta_{k'p}\delta_{kk'} + U_{kk'}\delta_{k'p}G_k{}^{H}(k,p) \tag{6.73}$$

where

$$U_{kk'} = -\left(\frac{i\beta}{2N}\right)^2 \sum_{\ell,\ell'} J_{k'\ell}\Lambda_{\ell'k}\hat{G}(\ell',\ell) \tag{6.74}$$

for s and p wave scattering only $U_{kk'}$ is given by

$$U_{kk'} = \frac{i\beta}{4N}\left(A_o + A_1 \cos\theta_{kk'}\right) \tag{6.75}$$

with

$$A_o = \frac{J_o\eta^o}{1+\xi_o} \qquad A_1 = \frac{\frac{1}{3}J_1\eta^1}{1+\frac{1}{3}\xi_1} \tag{6.76}$$

and

$$H(k,p) = U_{pk} + \sum_{p'} U_{p'k}U_{p'p}G_{p'} + \sum_{p',p''} U_{p'k}U_{p''p'}U_{p'p}G_{p'}G_{p''} + \cdots$$

$$= \frac{i\beta}{4N}\left[\frac{A_o}{1+\frac{1}{4}A_oF} + \frac{A_1\cos\theta_{kp}}{1+\frac{1}{12}A_1F}\right] \qquad (6.77)$$

Thus, from Fig. 18(b)

$$U_{kk'}\tilde{G}_{k'k}(\omega_n) = \sum_p U_{kk'}\delta_{k'p}[\delta_{kk'} + G_kH(k,p')]\bar{G}_{p'k'}$$

i.e.

$$\tilde{G}_{k'k}(\omega_n) = [\delta_{kk'} + G_kH(k,k')]\bar{G}_{k'k'} \qquad (6.78)$$

Now, in the lowest order approximation, we have

$$f(\Omega_n) = \frac{\gamma_o}{[|\omega_n| + \Delta_{(o)}]} + \frac{\gamma_1}{[|\omega_n| + \Delta_{(i)}]} \equiv f(\omega_n) \qquad (6.79)$$

and using the self-consistency relations (6.65) and (6.66), we get

$$A_o = \frac{\alpha^{(o)}J_o}{i\omega_n} \quad \text{and} \quad A_1 = \frac{\alpha^{(1)}J_1}{i\omega_n} \qquad (6.80)$$

Then, on simplification $\tilde{G}_{k'k}$ becomes

$$\tilde{G}_{k'k}(\omega_n) = G_k(\omega_n)\delta_{kk'} + \frac{\beta}{Nc}G_k(\omega_n)G_{k'}(\omega_n)[f^{(o)}(\omega_n) + f^{(1)}(\omega_n)\cos\theta_{kk'}]\text{sign }\omega_n$$

(6.81)

where

$$f^{(o)}(\omega_n) = \frac{\gamma_o}{|\omega_n| + \Delta_{(o)}} \text{ and } f^{(1)}(\omega_n) = \frac{\gamma_1}{|\omega_n| + \Delta_{(1)}} \qquad (6.82)$$

Now, since $V_{kk'} = \sum_p J_{pk'} n_{kp} - \frac{1}{2} J_{kk'} \equiv V_{(o)}(k) + V_1(k)\cos\theta_{kk'}$

equating the coefficients, we obtain

$$V_{(o)}(k) = -iJ_o \sum_{\omega_n} e^{i\omega_n 0^+} G_k(\omega_n) \left[1 + \frac{\beta}{Nc} f^{(o)}(\omega_n) \text{sign } \omega_n \sum_p G_p \right] - \tfrac{1}{2} J_o \qquad (6.83)$$

and

$$V_{(1)}(k) = -iJ_1 \sum_{\omega_n} e^{i\omega_n 0^+} G_k(\omega_n) \left[1 + \frac{1}{3} \frac{\beta}{Nc} f^{(1)}(\omega_n) \text{sign } \omega_n \sum_p G_p \right] - \tfrac{1}{2} J_1 \qquad (6.84)$$

Substituting these Eqs. in Eqs. (6.65) and (6.66), and solving the integral equations, one can obtain the temperature dependence of $\Delta_{(o)}$ and $\Delta_{(1)}$. We notice that the resulting integral equations are independent of each other and exactly similar in structure. Since the same equation for $\Delta_{(o)}$, for s-scattering only has been solved by Nagaoka (results are quoted in Chapter 3), we shall not go into any further detail.

Now, at low temperatures, $T < T_k$, current is given by, as usual

$$j_\mu = -\frac{2\pi}{3\beta} \frac{e^2}{m^{*2} v} A_\mu k_F^2 \rho \, \xi(\omega_p) \qquad (6.85)$$

where, in the lowest approximation, we take $\Omega_n = \omega_n$ and get

$$\xi(\omega_p) = \sum_{-\omega_p<\omega_n<o} \frac{1}{\omega_p + f(\omega_n) + f(\omega_n+\omega_p)} \tag{6.86}$$

Transforming this into contour integral and making analytic continuation, we obtain

$$\xi(-i\omega) = \frac{\beta}{2\pi i} \int \frac{dx}{e^{\beta x}+1} \left\{\phi(x) - \phi(x-\omega)\right\} \tag{6.87}$$

with

$$\phi(x) = \frac{1}{\left\{-i\omega + \frac{\gamma_o}{(ix+\Delta_{(o)})} + \frac{\gamma_1}{(ix+\Delta_{(1)})} + \frac{\gamma_o}{(-ix-i\omega+\Delta_{(o)})} + \frac{\gamma_1}{(-ix-i\omega+\Delta_{(1)})}\right\}} \tag{6.88}$$

In the d.c. limit,

$$\xi(-i\omega) \cong -\frac{i\beta\omega}{2\pi} \int \phi(x)\Big|_{\omega=o} \left(-\frac{\partial f}{\partial x}\right) dx$$

$$= \frac{i\beta\omega}{2\pi} \int \frac{(x^2+\Delta^2_{(o)})(x^2+\Delta^2_{(1)})}{2[\gamma_o\Delta_{(o)}(x^2+\Delta^2_{(1)})+\gamma_1\Delta_1(x^2+\Delta^2_{(o)})]} \left(-\frac{\partial f}{\partial x}\right) dx \tag{6.89}$$

At absolute zero temperature, the derivative of Fermi function can be replaced by a delta function and we get

$$\xi(-i\omega) = -\frac{i\beta\omega}{2\pi} \frac{\Delta_{(o)}\Delta_{(1)}}{2[\gamma_o\Delta_{(1)} + \gamma_1\Delta_{(o)}]} \tag{6.90}$$

and the conductivity, σ is

$$\sigma = \frac{1}{3} \frac{e^2}{m^{*2}v} k_F^2 \rho \quad \frac{\Delta_{(o)}\Delta_{(1)}}{2[\gamma_o \Delta_{(1)} + \gamma_1 \Delta_{(o)}]}$$

Putting back the values of γ_o, γ_1, $\Delta_{(o)}$ and $\Delta_{(1)}$ one finds

$$\sigma = \frac{ne^2}{m^*} \frac{\pi\rho}{8cN} \tag{6.91}$$

Hence, we see, at T = 0, inclusion of p-wave scattering reduces the conductivity to $\frac{1}{4}$ of its previous value. As temperature increases, we can write,

$$\xi(-i\omega) = - \frac{i\omega\beta}{2\pi} \frac{\pi\rho}{2cN} \int \frac{dy}{\frac{[\beta\Delta_{(o)}]^2}{y^2+[\beta\Delta_{(o)}]^2} + \frac{3[\beta\Delta_{(1)}]^2}{y^2+[\beta\Delta_{(1)}]^2}} \frac{e^y}{(1+e^y)^2} \tag{6.92}$$

Let, $\beta\Delta_{(o)} >> 1$, $\beta\Delta_{(1)} >> 1$, then expanding one obtains

$$\xi(-i\omega) = - \frac{i\omega\beta}{4\pi} \frac{\pi\rho}{cN} \int \frac{dy}{1 - \frac{y^2}{[\beta\Delta_{(o)}]^2} + 3\left[1 - \frac{y^2}{[\beta\Delta_{(1)}]^2}\right]} \frac{e^y}{(1+e^y)^2}$$

$$\cong - \frac{i\omega\beta}{16\pi} \frac{\pi\rho}{cN} \int \frac{dy}{1 - \frac{1}{4}\left[\frac{1}{[\beta\Delta_{(o)}]^2} + \frac{3}{[\beta\Delta_{(1)}]^2}\right] y^2} \frac{e^y}{(1+e^y)^2} \tag{6.93}$$

Expanding, once more

$$\xi(-i\omega) = -\frac{i\omega\beta}{2\pi}\frac{\pi\rho}{8cN}\int dy\left\{1+\tfrac{1}{4}y^2\left[\left(\frac{T}{\Delta_{(o)}}\right)^2+3\left(\frac{T}{\Delta_{(1)}}\right)^2\right]\right\}\frac{e^y}{(1+e^y)^2}$$

This gives the conductivity, σ, given by

$$\sigma = \sigma_o\left\{1+\frac{\pi^2}{12}\left[\left(\frac{T}{\Delta_{(o)}}\right)^2+3\left(\frac{T}{\Delta_{(1)}}\right)^2\right]\right\} \tag{6.94}$$

where $\sigma_o = \sigma$ at $T = 0$ and we found

$$\int y^2\frac{e^y}{(1+e^y)^2}\,dy = \frac{\pi^2}{3}$$

We consider the case $\Delta_{(1)} << \Delta_{(o)}$, i.e. the case of weak p wave scattering. With $\beta\Delta_{(o)} >> 1$, $\beta\Delta_{(1)} >> 1$, σ, becomes

$$\sigma \cong \sigma_o\left[1+\frac{\pi^2}{4}\left(\frac{T}{\Delta_{(1)}}\right)^2\right] \tag{6.95}$$

which is independent of $\Delta_{(o)}$, i.e. conductivity depends on the p-wave scattering only. In other words, p-wave scattering becomes important. By simple extension of the argument, one may say that other partial wave scattering are also important is this limit.

For, $\Delta_{(1)} << \Delta_{(o)}$ and when $\beta\Delta_{(o)} >> 1$ but $\beta\Delta_{(1)} << 1$, we go back to Eq. (6.92) and approximate

$$\xi(-i\omega) = -\frac{i\omega\beta}{4\pi}\frac{\pi\rho}{cN}\int\frac{dy}{\dfrac{1}{1+\dfrac{y^2}{[\beta\Delta_{(o)}]^2}}+\dfrac{3}{1+\dfrac{y^2}{[\beta\Delta_{(1)}]^2}}}\frac{e^y}{(1+e^y)^2}$$

$$\approx -\frac{i\omega\beta}{4\pi}\frac{\pi\rho}{cN}\int dy\left\{1+\left[\frac{y}{\beta\Delta_{(o)}}\right]^2\right\}\frac{e^y}{(1+e^y)^2} \tag{6.96}$$

And this gives

$$\sigma = \sigma_o\left[1+\frac{\pi^2}{3}\left(\frac{T}{\Delta_{(o)}}\right)^2\right] \tag{6.97}$$

In terms of resistivity Eqs. (6.95) and (6.97) can be written as (for $\Delta_{(1)} << \Delta_{(o)}$)

$$R(T) = R_o\left[1+\frac{\pi^2}{4}\left(\frac{T}{\Delta_{(1)}}\right)^2\right]^{-1} \quad (\beta\Delta_{(o)} >> 1,\ \beta\Delta_{(1)} >> 1) \tag{6.98}$$

and

$$R(T) = R_o\left[1+\frac{\pi^2}{3}\left(\frac{T}{\Delta_{(o)}}\right)^2\right]^{-1} \quad (\beta\Delta_{(1)} << 1,\ \beta\Delta_{(o)} >> 1) \tag{6.99}$$

where we denoted $1/\sigma_o = R_o$. Also with no assumption about the relative size of $\Delta_{(o)}$ and $\Delta_{(1)}$,

$$R(T) = R_o\left\{1+\frac{\pi^2}{12}\left[\left(\frac{T}{\Delta_{(o)}}\right)^2+3\left(\frac{T}{\Delta_{(1)}}\right)^2\right]\right\}^{-1} \tag{6.100}$$

The important thing to notice is that inclusion of p-wave scattering reduces the conductivity at T = 0 to one quarter of its value which we obtained in Chapter 3 for s-wave scattering only (see Eq. (6.91) . For weak p-wave scattering, $\Delta_{(1)} << \Delta_{(o)}$ only p-wave scattering is important for $\beta\Delta_{(o)} >> 1$, $\beta\Delta_{(1)} >> 1$ and only s-wave scattering is significant when $\beta\Delta_{(o)} >>$ but $\beta\Delta_{(1)} << 1$.

6.5 Discussion

The most important conclusion we have arrived at in this chapter concerns the high temperature behaviour of the Kondo system. Inclusion of vertex corrections, for the extended exchange interaction formulation, gave rise to correction, third order in exchange interaction and appeared in the coefficient of the leading ℓn term. We showed that for a particular ratio of the strengths of the s and p wave scattering, this coefficient can vanish, giving a different type of high temperature behaviour. From our results in Section 6.3, if we write the expression for resistivity, R(T)

$$R(T) \cong cR_m [1 + \alpha\lambda + \beta\lambda^2] \tag{6.101}$$

where, $\lambda = \rho J/N\ell n\ T/D$, α, β are constants such that $\alpha\lambda$, $\beta\lambda^2 << 1$. R_m is the resistivity in the first Born approximation, and c is the concentration of impurities. At high temperatures, we have $\alpha\lambda > \beta\lambda^2$ and if we call the reverse situation, i.e. $\alpha\lambda < \beta\lambda^2$ 'low' temperature region, we can define a critical temperature, T_c given by

$$\frac{T_c}{D} = \left[\frac{T_k}{D}\right]^{\alpha/\beta} \tag{6.102}$$

where, T_k is the Kondo temperature. Then for $\alpha/\beta << 1$, $T_k << T_c$. To ignore the leading ℓn term, $\alpha\lambda$, in the resistivity expression (6.101), we need $\alpha/\beta << 1$. Thus, we have a temperature region, given by

$$T_k << T << T_c \tag{6.103}$$

where our formulation is applicable. The Eq. (6.101) is valid for $T >> T_k$ and if we take $D \sim 10^5$K, $T_k \sim 10^{-5}$K and $\alpha/\beta \sim 10^{-1}$, T_c becomes of the order of 10^4K. Also, if $T_k \sim 10^\circ$K, $D \sim 10^5$K and $\alpha/\beta \sim \frac{1}{4}$, T_c is again 10^4K. Hence, we can, in principle have a large temperature region for which our theory is applicable. For normal Kondo effect, we have $T >> T_k$ and $T >> T_c$. For $T >> T_c$, the leading ℓn-term dominates, no matter how small α is and also even if α is of the order of β . But, in the latter case, $T_k \sim T_c$.

Experimentally, the resistivity of RhFe[74], IrFe[75], PtFe[76] and PdCo[76] alloys does not show a minimum. For RhFe the resistivity was found to increase gradually with temperature and at about 20°K, it bends in the shape of a knee and then rises sharply with temperature (for 0.1 at % of Fe concentration). For higher concentration this knee disappears giving a very sharp rise with temperature. For IrFe, strong temperature dependence of resistivity was found for 0.01 at % concentration of Fe. Similar behaviour was also found for PdCo alloys. These alloys have been called 'Coles alloys' and attempts have been made to explain their behaviour. Loram et al. found that their data on PdCo alloy for excess resistivity, $\Delta\rho$ agree well with an expression $\Delta\rho = A + B\ell nT$, where B was positive. But, to account for their magnetoresistance data, a large positive, but improbable value of the exchange coupling between conduction electrons and local spins is required. Rivier and Zlatic[80] attempted to explain these results from the 'localized spin fluctuation' point of view. It has been argued[95] that since these alloys contain transition elements for both host and

impurity, they are not Kondo systems with well defined localized states. But, susceptibility data[77], specific heat[79] anomaly at low temperatures, also Mössbauer anomalies[79] similar to that in CuFe alloy, all indicate that these alloys behave like a Kondo system with negative exchange interation, except for resistivity.

We have shown that for alloys having strong p-wave scattering, the logarithmic behaviour in the resistivity due to exchange scattering will be smeared and in the extreme case will vanish totally. This resistivity will tend to a constant and when combined with residual resistivity and resistivity due to lattice scattering ($\propto T^5$) the total resistivity will show no resistance minimum and a sharp rise with the temperature is inevitable. But detailed comparison with experimental data has proved problematic. Firstly, the magnitude of J itself is controversial[93]. Since the Kondo temperature T_k depends exponentially on the exchange constant J, a small change in J can vary T_k by an enormous amount. Secondly, fixing the ratio of J_o and J_1 will be totally arbitrary. Finally, it has been suggested[94] that these alloys are not systems with strong p-wave scattering. Therefore, we prefer to wait until a better understanding of the problem has been achieved.

CHAPTER 7 CONCLUSION

In this thesis, we have applied the linear response formalism to calculate the electrical conductivity of dilute magnetic alloys and used the s-d exchange Hamiltonian throughout. Since this Hamiltonian can be derived from the Anderson Hamiltonian, (physically, not very much different from the Wolff model), under special circumstances and since both of the models were shown to produce a Kondo singularity[97] for the electrical resistivity and Curie-Weiss law[98] for the magnetic susceptibility, it is expected that the results derived in one model would not be very much different for the other. It must be emphasized here that one is not at all certain whether or not the s-d exchange model is adequate for treating the dilute magnetic alloys. Considerable efforts have been made to study the Anderson and Wolff models where the magnitude of the impurity spin is not assumed to be fixed but is allowed to vary. It has been known for a long time that a model with a fixed half integral or integral impurity spin cannot describe these alloys rigorously, since the spin values derived from the high temperature susceptibility are generally not equal to half or any multiple of it. This leads one back to the alternative approach to the problem, viz. the problem of the existence and stability of an impurity spin in a metallic environment, as separate from the way this spin interacts with the conduction electrons. Perhaps, it will be profitable to study both of these problems together.

Instead of the usual single impurity formulation, we have formulated the equations of motion with N_i impurities

distributed randomly throughout the system. It was necessary for us to do so in order to apply linear response theory. But, in effect, we have neglected the impurity-impurity correlations by taking the average over the impurity sites before solving the equations of motion. It is a standard practice for the low concentration of impurities. The interaction between impurities brings in many new effects. These have been investigated by several authors[99], but the problem is not well understood yet.

In our calculations, the ordinary potential scattering has not been included. It was shown by Kondo[100] that the ordinary scattering has no essential effect on the thermodynamic properties of the system. But, for the transport properties it was thought to have severe effects. The giant thermoelectric power was explained as a result of the combined effect of the ordinary and exchange scattering. Fischer[101] investigated the effect of the ordinary scattering on the exchange scattering and found a factor $\cos^6\eta_\ell \cos 2\eta_\ell$ (η_ℓ are phase shifts) incorporated in the leading logarithmic term. Since, this factor becomes negative when $\eta_\ell > \pi/4$, the $\ell n T$ term can change sign. But this result does not agree with that of Abrikosov[47] who found no change in the temperature-dependent resistivity due to normal scattering.

There are two ways to take the potential scattering into account. First, one can add on additional term containing the ordinary potential to the Kondo Hamiltonian[101-104] and then adopt Nagaoka's decoupling scheme to solve the equations. Let us call the resultant t-matrix for non spinflip scattering, t_{J+V}. Alternatively, one can make use of a canonical transformation[102] to eliminate the potential term. In that case

the exchange coupling constant, J is replaced by a renormalized coupling constant, $\tilde{J}$. Then one can apply the same decoupling scheme to obtain the corresponding t-matrix, $t_{\tilde{J}}$. It was shown by Schotte[105] that these two t-matrices are related by $t_{J+V} = t_{\tilde{J}} e^{2i\delta_V} + t_V$, where t_V and δ_V are the t-matrix and the phase shift due to the ordinary potential scattering only. Thus it is clear that one need not include the ordinary potential explicitly in the formulation of the Kondo problem.

Recently, scaling techniques[106] have been applied to develop a theory for the Kondo system which is valid at all temperature regions. There, Anderson, Yuval and Hamann showed that the Kondo problem is equivalent to a certain type of one dimensional statistical problem and solved that problem by deriving scaling laws connecting solutions for different sets of parameters with each other. Despite this progress, there are no quantitative theoretical predictions for quantities like resistivity, low temperature susceptibility or specific heat. Furthermore, the theory includes s-wave scattering only.

In calculating the conductivity of the system we used the Kubo formula[86] of linear response. When the electrons in a metal are subjected to the sort of scattering that can be described by an isotropic relaxation time, then the Kubo formula becomes the quasi classical expression as derived from the Boltzmann transport equation. But for more complicated scattering mechanism, like that in a Kondo system, it is not at all clear from the start that one can use a simple relaxation time. Our calculations (Chapters 2 and 3) confirm the contention that the scattering in a Kondo system,

as far as it is described by the s-d model can be represented by a simple relaxation time.

Our analytic expressions for the complex conductivity (Chapter 4) at low temperatures may serve as a useful starting point for future investigations. Moriya and Inoue[90] have sugeested that the experimental measurements of the surface impedance of Kondo alloys at low temperatures in the microwave or far infrared frequency regions might differentiate the lsf and the s-d models. Both the theories show a significant deviation from the Drude model, and for special cases, somewhat different behaviour is predicted for the two models. Both theories predict peaks in the frequency-dependent conductivity, but the ones in the lsf model are sharper. Our theory, valid for frequencies very much less than 10^{12}Hz, does not predict any peak. Unfortunately, there are no experimental results available at the moment which would permit any definite conclusion about these predictions.

Our most important contribution to the theories of Kondo systems is the finding of the effect of inclusion of p wave scattering of the exchange interaction (Chapters 5 and 6). The correction to the leading logarithmic term is found as a result of including the vertex corrections which arise from the non-conservation of local charges. As had been found for the BCS theory[45] of superconductivity, the quasi-particle excitations, if treated independently, do not conserve charge. Mathematically, the situation arises when the two-particle Green's function is replaced by a product of two single-particle Green's functions. In the Kondo problem, one also decouples the higher order Green's function to the lower order ones. Hence the problem of non conserva-

tion of charge is present unless one works within a conserving approximation. One way to ensure the conservation laws, when calculating the response of the system to an electric field, is to make use of a 'generalized Ward's identity'[107] which is the Green's function analogue of the continuity equation. Using this identity, we found the correction term in the high temperature conductivity of the Kondo system. The effect of this term can in fact be very severe.

We have had difficulty in finding experimental data for alloys in which p wave scattering would be strong. We expect p-wave scattering to be important for large impurities with a finite range of interaction; s-wave scattering assumes a contact type of interaction described by a delta-function. The high temperature resistivity of alloys of second or third row transition-metal hosts with a small amount of first row transition-metal impurities may show agreement with our theory. These alloys showed two distinct types of properties. One category exhibits well-defined impurity moments and they undergo magnetic ordering at low temperatures. They also show a negative magnetoresistance. PdFe[108] and MoFe[109] alloys are typical examples of this type. The second category does not show magnetic ordering and it has an effective moment per impurity which decreases at low temperatures. The resistivity has a positive temperature dependence; the magnetoresistance is found to be positive. RhFe[74], IrFe[75] etc., show such behaviour. But experimental investigations on some other alloys like PtFe[76], PdFe[76] etc., showed some behaviour common to both categories.

Attempts, along several different lines, have been made to explain the two types of behaviour exhibited by the alloys named earlier but none of them can, as yet, claim complete success. Kondo[44] tried to describe these systems with a positive exchange interaction. But it was pointed out[48] that the decrease in moment at low temperatures as well as a large peak in the thermoelectric power in these alloys would not be possible from a positive J. A number of authors attempted to explain these systems taking ordinary potential scattering into account. But the residual resistivity[110] of these alloys did not support this contention. Knapp[81] has suggested a two-band model for the purpose, but there again, one can reject this on the grounds that it would not produce a large thermoelectric power[111]. Yet another approach is through the localized spin fluctuation (lsf) model[80]. The situation, at present is by no means clear, as no single theory could explain any substantial number of properties over a reasonable temperature range.

From our calculations, we have found that the inclusion of p-wave scattering can change the logarithmic temperature dependence of the resistivity at high temperatures and in the extreme case the ℓnT term can vanish totally. This term then added to the residual resistivity and the resistivity due to the lattice scattering (αT^5) gives no resistance-minimum but a sharp rise in the resistivity as temperature increases. This may serve as a basis for explaining the behaviour of RhFe and related alloys. As more and more experimental data are becoming available, we hope our calculations will throw some light on the complicated scattering mechanisms in these alloys.

Our calculations, even if they are found to have no relevance to typical Kondo alloys, (those with definite magnetic moments), can, we believe, be a basis for the investigation of the transport properties of alloys, with large magnetic impurities, where p-wave scattering in the exchange interaction is expected to be important, The expression for high temperature resistivity developed in the present thesis can, in fact, predict the temperature dependence of the resistivity for the relevant alloys. In future, it would be of interest to solve the equations for all partial waves and see how the results are modified. A straightforward calculation, along similar lines, for the Anderson model, might clear up the physical situation.

The vertex corrections need to be included in the expression for low temperature resistivity. This may be attempted in future. One might use the conserving approximations developed by Kadanoff and Baym[112] to carry out the calculations. Future work can be directed along these lines.

Appendix A

In Chapter 3, we evaluated the restricted ω_n-sum by using the contour integral method. Using the standard result

$$\sum_{\omega_n} f(\omega_n) = \frac{-\beta}{2\pi i} \int_{c'} \frac{dz}{e^{\beta z}+1} \; f(-iz) \tag{A.1}$$

where the contour c' surrounds the poles of a function which has simple poles at values $i\omega_n$, we obtained [See Eqs.(3.44) and (3.47)],

$$\xi(\omega_p) = \sum_{-\omega_p < \omega_n < o} \frac{1}{\omega_p + \dfrac{\gamma}{1-b\ell n \dfrac{\omega_n+\omega_p}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{-\omega_n}{D}}}$$

$$= \frac{\beta}{2\pi i} \int \frac{dz}{e^{\beta z}+1} \; \frac{1}{\omega_p + \dfrac{\gamma}{1-b\ell n \dfrac{\omega_p - iz}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{iz}{D}}}$$

$$- \frac{\beta}{2\pi i} \int \frac{dz}{e^{\beta z}+1} \; \frac{1}{\omega_p + \dfrac{\gamma}{1-b\ell n \dfrac{-iz}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{\omega_p + iz}{D}}}$$

This is true only if (i) the end parts of the contour (Fig.9) do not contribute and (ii) the integrand has no poles within the contour.

The contribution from the right hand side end part (from $\infty - i\omega_p$ to ∞) vanishes, because the Fermi factor gives

zero for large positive value of z. Since the function $\xi(\omega_p)$ tends to ω_p^{-1} as $\omega_n \to \infty$, the contribution from the left hand side does not vanish. By considering the sum more carefully, we shall show that this does not contribute any correction of interest.

If we subtract ω_p^{-1} from the start, the integrand will be absolutely convergent and the end parts would not contribute. Therefore, we have

$$\xi(\omega_p) = \sum_{-\omega_p<\omega_n<0} \left\{ \frac{1}{\omega_p + \dfrac{\gamma}{1-b\ell n \dfrac{\omega_n+\omega_p}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{-\omega_n}{D}}} - \frac{1}{\omega_p} + \frac{1}{\omega_p} \right\} \qquad (A.2)$$

Transforming this to the contour integral form and making the analytic continuation, we obtain

$$\xi(-i\omega) = \frac{\beta}{2\pi} + \frac{\beta}{2\pi i} \int \frac{dx}{e^{\beta x}+1} \left\{ \frac{1}{-i\omega + \dfrac{\gamma}{1-b\ell n \dfrac{ix}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{-ix-i\omega}{D}}} \right.$$

$$\left. - \frac{1}{-i\omega + \dfrac{\gamma}{1-b\ell n \dfrac{ix-i\omega}{D}} + \dfrac{\gamma}{1-b\ell n \dfrac{-ix}{D}}} \right\} \qquad (A.3)$$

$$\equiv \frac{\beta}{2\pi} + \frac{\beta}{2\pi i} \int f(x)g(x)dx \qquad (A.4)$$

where f(x) is the Fermi function and the function g(x) is defined from (A.3). We notice that the function g(x) is odd and so we can write (A.4) in the following form

$$\xi(-i\omega) = \frac{\beta}{2\pi} + \frac{\beta}{2\pi i}\int_0^\infty (2f(x) - 1)g(x)dx \qquad (A.5)$$

The next step is to evaluate the integrals. We write

$$\int_0^\infty g(x)dx = \lim_{L\to\infty}\int_0^L g(x)dx$$

$$= \lim_{L\to\infty}\int_0^L [\phi(x) - \phi(x-\omega)]dx \qquad (A.6)$$

where

$$\phi(x) = \frac{1}{-i\omega + \dfrac{\gamma}{1-b\ell n\,\dfrac{ix}{D}} + \dfrac{\gamma}{1-b\ell n\,\dfrac{-ix-i\omega}{D}}} \qquad (A.7)$$

From (A.6), we get

$$\int_0^L g(x)dx = \int_{L-\omega}^L \phi(x)dx - \int_{-\omega}^0 \phi(x)dx$$

$$= \int_0^\omega \phi(L-\omega)dx - \int_{-\omega}^0 \phi(x)dx \qquad (A.8)$$

Now, for large L we can expand the ℓn terms appearing in $\phi(x)$ to get

$$\ell n\,\frac{L-x}{D} \cong \ell n\,\frac{L}{D} - \frac{x}{L}$$

and

$$\ell n\,\frac{L-x+\omega}{D} \cong \ell n\,\frac{L}{D} - \frac{x-\omega}{L} \quad .$$

Then the first integral in (A.8) gives i as $L \to \infty$.

The other integral in (A.5) can be written as

$$\int_0^\infty f(x)g(x)dx = \int_0^\infty [\phi(x,\omega) - \phi(x-\omega,\omega)]f(x)dx \qquad (A.9)$$

where the function $\phi(x,\omega)$ is given by (A.7). From (A.9), one obtains

$$\int_0^\infty f(x)g(x)dx = \int_0^\infty \phi(x,\omega)[f(x)-f(x+\omega)]dx - \int_{-\omega}^0 \phi(x,\omega)f(x+\omega)dx$$

$$\cong -\omega \int_0^\infty \phi(x,\omega)\,\frac{\partial f}{\partial x}\,dx - \int_{-\omega}^0 \phi(x)f(x)dx \qquad (A.10)$$

In the d.c. limit, the first integral is evaluated to be

$$\frac{1}{2\gamma} - \frac{b}{2\gamma}\ell n\left|\frac{T}{1.13D}\right|$$

and the second integral cancels the second integral in (A.8) in the d.c. limit when inserted in (A.5). The factor i coming from the first integral of (A.8) cancels the first term in (A.5). Therefore, we get

$$\xi(-i\omega) = \frac{i\omega\beta}{4\pi\gamma}\left[1 - b\ell n\left|\frac{T}{1.13D}\right|\right] \qquad (A.11)$$

which is exactly the same as Eq. (3.53). Hence, neglection of the contribution from the end part of the contour is justified. It may be mentioned here that the first part of the integral in (A.10) has another part higher order in b.

A careful evaluation of that term will make it clear that the contribution coming from there is essentially of $O(J^4)$ and higher and hence of no interest to us. A similar treatment can be applied to all other evaluations of ω_n-sums in this thesis.

The second point we want to resolve is whether the integrand of Eq. (3.44) has any pole within the contour. That the integrand has no pole within the contour can be shown quite easily if we recall the approximation made in Eq. (3.40). If we had not made that assumption we could write

$$\xi(\omega_p) = \sum_{-\omega_p<\omega_n<o} \frac{1}{\omega_p + \dfrac{\gamma}{1-b\ell n \dfrac{\omega_n^2}{\omega_n^2+D^2}} + \dfrac{\gamma}{1-b\ell n \dfrac{(\omega_n+\omega_p)^2}{(\omega_n+\omega_p)^2+D^2}}} \tag{A.12}$$

Expanding this expression for $b \ll 1$, we get

$$\xi(\omega_p) = \sum_{-\omega_p<\omega_n<o} \left\{ \frac{1}{(\omega_p+2\gamma)} - \frac{\gamma b}{(\omega_p+2\gamma)^2} \ell n \left[\frac{\omega_n^2}{(\omega_n^2+D^2)} \frac{(\omega_n+\omega_p)^2}{(\omega_n+\omega_p)^2+D^2} \right] \right\} \tag{A.13}$$

One can easily verify that the expansion does not violate the analyticity requirements[113] of the summand. If now we write the ω_n-sum into a contour integral form in the same way as we have done in Chapter 3, it becomes trivial to show that the integrand has no pole within the contour. The integrand has a pole within the contour only if the argument

of ℓ_n either vanishes or tends to infinity there. But it is so only for values $z = o$, $z = D$, $z = i\omega_p$ and $z = D-i\omega_p$ and none of these values lies within the contour. Therefore the integrand has not got any pole within the contour.

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