

AN ABSTRACT OF THE THESIS OF

Narsingh R. Bharatiya for the degree Doctor of Philosophy

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in Dilute Non-Magnetic Alloys.

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First the theory of electron-phonon contributions to the de Haas-van Alphen effect in normal systems (pure metals in the non-superconducting state) is reviewed. Then a new derivation of the de Haas-van Alphen oscillations for an interacting system is given. The result is applied to electron-phonon scattering to show that contrary to what might be expected, the Dingle temperature does not include electron-phonon scattering effects and, under reasonable approximations, indeed one again recovers the quasi-particle formula for the amplitude in the interacting system; however, with the electron-phonon enhanced mass replacing the bare electron (free or band) mass. Also a calculation of the electron-phonon scattering in dilute non-magnetic alloys is presented in which an uncorrelated ensemble average of phonon Green's functions for the disordered system is used. It is found that for the extended 'high temperature limit' derived above the various contributions to the normal electron self-energy (relevant to the dHvA effect) still

have a linear temperature dependence. However, the electron-phonon mass enhancement factor λ now depends on two more parameters besides the effective mass of the electrons in the host.

Electron-Phonon Interactions and de Haas-van Alphen
Effect in Dilute Non-Magnetic Alloys

by

Narsingh Ramniwas Bharatiya

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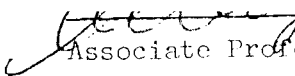
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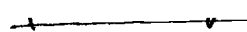
Redacted for Privacy


Associate Professor of Physics

Redacted for Privacy

Chairman Department of Physics

Redacted for Privacy


Dean of Graduate School

Date thesis is presented August 5, 1976

Typed by Narsingh for Narsingh R. Bharatiya

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ELECTRON-PHONON INTERACTIONS AND DE HAAS-VAN ALPHEN EFFECT IN DILUTE NON-MAGNETIC ALLOYS.

1. INTRODUCTION

The de Haas-van Alphen effect (dHvA), discovered in 1930, has by now become one of the most powerful tools in the study of Fermi surfaces of metals and alloys as well as properties of electrons moving on the Fermi surface. Whereas, measurements of oscillation frequencies give the cross-sectional area of extremal orbits which ultimately yield the size and shape of the Fermi surface, amplitude measurements provide much valuable information regarding the many body interactions. In this study we focus our attention on the electron phonon interactions in general and those in dilute alloys in particular.

Let us first consider the case of a free electron gas in a magnetic field. As shown in appendix A, the oscillatory effect arises because of the quantization of the free electron states due to the magnetic field. The thermodynamic potential Ω of the degenerate free electron gas in the magnetic is given by⁽²⁵⁾

$$\Omega = - \frac{(m \omega_c)^{3/2}}{\pi^2 \beta} \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \frac{\cos \left(\frac{2\pi\mu}{\omega_c} \pm \frac{\pi}{4} \right) \cos \left(\frac{\pi g \mu_B r B}{\omega_c} \right)}{\sinh \left(\frac{r \pi^2 k_B T}{\omega_c} \right)} \quad (1.1)$$

where all symbols used are defined in chapter II as well as in appendix C. From this, to a good approximation, the magnetization is given by

$$M = - \frac{2m \omega_c^{1/2} \mu}{\pi \beta B} \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{1/2}} \frac{\sin\left(\frac{2\pi r \mu}{\omega_c} \pm \frac{\pi}{4}\right) \cos\left(\frac{\pi g \mu_B r B}{\omega_c}\right)}{\sinh\left(\frac{r \pi^2 k_B T}{\omega_c}\right)} \quad (1.2)$$

As is evident, there is an oscillatory behaviour in $(1/B)$ with frequency f , proportional to the extremal cross-sectional area of the Fermi surface, given by

$$f = \frac{mc \mu r}{e} \quad (1.3)$$

for the r -th harmonic. The amplitude of the r -th harmonic is dictated by the sinh term appearing in the denominator of eq.(1.2). The magnetic fields and temperatures commonly used in the dHvA experiments are such that $\frac{2\pi^2 k_B T}{\omega_c} \gg 1$. In such a situation the sinh term can be approximated as

$$A_r \sim \frac{1}{\sinh\left(\frac{\pi^2 k_B T r}{\omega_c}\right)} \approx e^{-\frac{2\pi^2 k_B T r}{\omega_c}} \approx e^{-\frac{2\pi^2 k_B T r (mc)}{(eB)}} \quad (1.4)$$

thus giving an exponential amplitude factor. From eq.(1.4) we see that, if we plot the logarithm of the amplitude vs. temperature, we get a straight line whose slope is proportional to the electron mass. In proceeding beyond the free electron approximation to include the crystal potential one may, in many simple metals, employ an effective mass approximation in which the bare electron mass is modified and called the band-mass.

In the derivation of above formulae the electron states are regarded as having infinite lifetimes. In the case that impurities are present, the electron states will acquire finite lifetime. This effect was considered in an earlier work by Dingle⁽³⁾ in which it was shown that if one introduces a Lorentzian broadening for the Landau levels then an additional term appears for the amplitude which is given by

$$A_r^{\text{imp}} \sim e^{-\frac{\pi \Gamma \Gamma}{\omega_c}} \quad (1.5)$$

where Γ is the Landau level width. Since according to Dingle $\Gamma = 2\pi k_B T_D$, it is possible to combine the two amplitude factors of eq.(1.4) and eq.(1.5) and write

$$A_r \sim e^{-\frac{2\pi^2 k_B \Gamma (\tau + T_D)}{\omega_c}} \quad (1.6)$$

where T_D is called the Dingle temperature.

The Dingle temperature "apparently" contains all the information about Landau level broadening. In fact this idea is actively pursued by experimental workers in this field in trying to understand the way in which electrons scatter as they move on the Fermi surface^(13,23).

Extending Dingle's arguments to include the scattering due to phonons one naively expects that as the temperature is raised from absolute zero, the population of phonons increases and therefore the amplitude of the oscillations should further decrease. Shoenberg⁽²⁶⁾ suggested that including the effects of phonon scattering the Dingle temperature should depend on temperature as

$$T_D = T_0 + \alpha T^3 \quad (1.7)$$

where estimates based on thermal conductivity suggest that $\alpha \simeq 10^{-2}$. Such a temperature dependence would be easy to find in a logarithmic plot of amplitude vs temperature; or the logarithmic plots of field dependence of amplitude at different temperatures. However, in the experiments done on mercury, where such effects are expected because of strong electron-phonon coupling in it, Palin⁽¹⁶⁾ found no such temperature dependence of the Dingle temperature for field strengths upto 100 kG. and temperatures upto 17° K.

In actual fact a much earlier work of Fowler and Prange⁽⁵⁾ involving a field theoretic study of the electro-phonon interactions, in the presence of magnetic field, predicted that the Dingle temperature would be temperature independent. However, it was strictly speaking a high temperature result and apparently was unknown to Shoenberg. An extension of the arguments of Fowler and Prange (FP) was made by Engelsberg and Simpson (ES)⁽⁴⁾ in which they attempt, by numerical analysis using superconducting tunneling data, to go beyond the FP high temperature limit. They suggest that at very low temperatures and extremely high fields some temperature dependence of the Dingle temperature might be expected. However, at these lower temperatures the rate of convergence of their series is poor and their conclusions may not be as reliable as one might hope.

In the present work we continue the investigation begun by FP and carried on by ES and develop an extension of FP high temperature result which is valid at lower temperatures.

In our result we find that contrary to ES prediction, it is very unlikely that one can see an amplitude of dHvA oscillations due to

phonon scattering which differs appreciably from the quasi-particle formula of eq.(1.2) except that now the electron-phonon enhanced mass should be used in place of bare electron(free or band) mass. Further more the result that we obtain has the advantage of being in a closed form in which the effects of the electron-phonon interactions are easily considered by calculating, according to the field theoretic prescriptions, irreducible self-energies corresponding to the electron-phonon interactions. We take advantage of the simplicity of this form for the dHvA formulation to investigate as well, the consequences of impurities in the form of a dilute substitutional alloy, on the dHvA effect. We consider the case of both static and dynamical lattice impurities which will modify the electron scattering. We also derive the result for fixed impurity scattering in the case that the electrons have been renormalized to include phonon scattering.

II. DE HAAS-VAN ALPHEN EFFECT IN INTERACTING SYSTEM.

2.1 General Formalism

The de Haas-van Alphen effect is an equilibrium thermodynamic effect in which one measures the magnetization \vec{M} of a metal or semi-metal. This can always be computed from the thermodynamic grand potential Ω , which in turn is defined by

$$\Omega = -\frac{1}{\beta} \ln Z_G \quad (2.1)$$

where Z_G is the grand partition function and $\beta = \frac{1}{(k_B T)}$; k_B is Boltzmann constant and T is the absolute temperature. By taking a derivative of Ω with respect to the magnetic field \vec{B} at constant temperature T and volume V , we arrive at the magnetization; i.e.

$$\vec{M} = -\left(\frac{\partial \Omega}{\partial \vec{B}} \right)_{T, V} \quad (2.2)$$

The computation of Ω , for an interacting system can not be done exactly and very often perturbation theory, as outlined in the following, is used.

Introducing a variable coupling constant g , one can write the Hamiltonian $H(g)$, of the interacting system, as

$$H(g) = H_0 + g H_1 \quad (2.3)$$

so that $g = 1$ describes the interacting system whereas $g = 0$ describes some simpler system. In terms of g , Ω is given by^(1,6)

$$\Omega = \Omega_0 \pm V(2S+1) \text{Tr} \int_0^1 \frac{dg}{g} \frac{1}{\beta \hbar} \sum_n \Sigma_g(\omega_n) G_g(\omega_n) \quad (2.4)$$

where,

Ω_0 = thermodynamic potential of the non-interacting system,

V = volume of the system,

S = spin quantum number of the particles,

$\hbar = h/2$,

h = Planck's constant,

$\omega_n = (2n + 1)\pi/\beta = (2n + 1)\pi k_B T$.

$G_g(\omega_n)$ is the exact Green's function for the interacting system and $\Sigma_g(\omega_n)$ is a quantity called proper self-energy which is related to the Green's function $G_g(\omega_n)$ by an integral equation which is

Dyson's equation

$$G_g(\omega_n) = G_0(\omega_n) + G_0(\omega_n) \Sigma_g(\omega_n) G_g(\omega_n)$$

where, $G_0(\omega_n)$ is the Green's function for the non-interacting system corresponding to H_0 . The $\omega_n = (2n + 1)\pi/\beta$ are points on the imaginary energy axis. This rather peculiar state of points on the imaginary energy axis is in fact not so peculiar when it is observed that the finite temperature Green's function is periodic along an imaginary time axis. Thus the Green's functions may be expanded in the usual manner and the ω_n merely represents the summation index for this Fourier series.

The plus sign in eq.(2.4) correspond to fermions whereas minus sign is taken for bosons. Thus for electrons we take positive sign, $s = 1/2$ and using the units such that $\hbar = 1$, we get from eq. (2.4)

$$\Omega = \Omega_0 + \frac{V}{\beta} \text{Tr} \int_0^1 \frac{dg}{g} \Sigma_g(\omega_n) G_g(\omega_n) \quad (2.5)$$

At this point it must be stated that the most general method of computing Ω is extremely complex and abstract. It arises from a paper by Yang and Lee⁽¹²⁾ and later recasted into the Green's function language by Luttinger and Ward⁽¹⁰⁾. However, it is possible to demonstrate reasonably clearly the basic elements of the general arguments by focusing on a simple situation, which is being done in what follows.

Rewriting the Dyson's eq.(2.3) as

$$G_g = G_0 + G_0 \Sigma_g G_0 + \dots \quad (2.6)$$

where, for convenience, we suppress all the functional dependences except that on the variable coupling constant g . By writing in the form of eq. (2.6) we have isolated the effects of interactions in the self-energy $\Sigma_g(\omega_n)$.

Using eq. (2.6), the product $\Sigma_g G_g$ can be written as

$$\Sigma_g G_g = \left(\Sigma_g + \Sigma_g G_0 \Sigma_g + \dots \right) G_0 \quad (2.7)$$

It is convenient to represent the various terms of the series of eq. (2.7) by Feynman diagrams. In particular the lowest order electron-phonon proper self-energy, Σ_g , can be represented by the Feynman diagram of fig. (2.1) where the solid line represents the electron Green's function $G_0(\omega_n)$ and the dotted line the phonon Green's function $d(\omega_n)$

The vertex represents the coupling constants between the electrons and phonons. [The form of the actual coupling constant is given in eq.(4.24) of chapter IV].



Fig. 2.1

Thus, in terms of Feynman diagram of fig. (2.1) we can represent the series in the parenthesis of eq. (2.7) as in fig.(2.2).

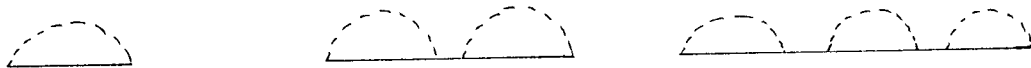


Fig.2.2

The G_0 , written outside the parenthesis in eq. (2.7), has the effect of closing the open diagrams of fig.(2.2), thus giving the diagrams of fig.(2.3) for the thermodynamic potential Ω .

However, the diagrams of fig.(2.3) can also be obtained by other irreducible self-energies besides those of fig.(2.2). These are shown in fig.(2.4).

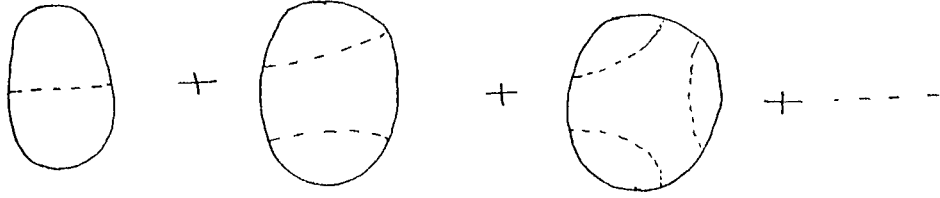


Fig. 2.3



Fig. 2.4

Thus, the summation of the diagrams of fig.(2.3) for the thermodynamic potential actually involves the summation of the two types of self-energy diagrams of fig.(2.3) and fig.(2.4). We note that there are two diagrams in all higher orders except the first, hence the series for

$\sum_g G_g$ can be written as

$$\begin{aligned}
 \sum_g G_g &= \sum_g G_0 + 2 \left(\sum_g G_0 \sum_g G_0 + \dots \right) \\
 &= 2 \left(\sum_g G_0 + \sum_g G_0 \sum_g G_0 + \dots \right) - \sum_g G_0 \\
 &= 2 \frac{\sum_g G_0}{1 - \sum_g G_0} - \sum_g G_0 \\
 &= 2 \frac{g^2 \sum G_0}{1 - g^2 \sum G_0} - g^2 \sum G_0
 \end{aligned}$$

(2.8)

since $\Sigma_g = g^2 \Sigma$ for second order interaction in coupling constant.

It may be noted here that the self-energy Σ still has an implicit dependence on the actual coupling constant for which we use the notation \bar{g} . That dependence is shown explicitly in later calculations, when we need the actual analytical form of Σ .

Using eq.(2.8) in eq.(2.5) we get

$$\Omega = \Omega_0 + \frac{V}{\beta} \text{Tr} \int_0^1 \frac{dg}{g} \left(\frac{g^2 \Sigma G_0}{1 - g^2 \Sigma G_0} \right) - g^2 \Sigma G_0 \quad (2.9)$$

Carrying out the integration over the variable coupling constant g , we get

$$\Omega = \Omega_0 + \frac{V}{\beta} \text{Tr} \left[-\ln(1 - \Sigma G_0) - \frac{1}{2} \Sigma G_0 \right] \quad (2.10)$$

From the standard Dyson's eq. for the Green's function

$$G = G_0 + G_0 \Sigma G \quad (2.11)$$

we get,

$$(1 - \Sigma G_0) = \frac{G_0}{G} \quad (2.12)$$

The thermodynamic potential for the non-interacting system is given by⁽¹⁰⁾

$$\Omega_0 = -\frac{V}{\beta} \ln \left(\left| \frac{1}{G_0} \right| \right) \quad (2.13)$$

Using eq.(2.12) and eq.(2.13), we can write eq.(2.10) as

$$\Omega = -\frac{V}{\beta} \text{Tr} \left[\ln \left(\left| \frac{1}{G} \right| \right) + \frac{1}{2} \sum G_o \right] \quad (2.14)$$

For the purpose of further generalization we write this as

$$\Omega = -\frac{V}{\beta} \text{Tr} \left[\ln \left(\left| \frac{1}{G} \right| \right) + \sum G_o \right] + \text{Tr} \frac{V}{2\beta} \sum G_o \quad (2.15)$$

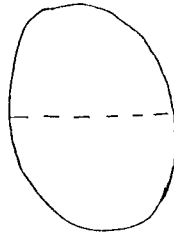


Fig. 2.5

Basically what we are doing is constructing a quantity

$$-\frac{V}{\beta} \text{Tr} \left[\ln \left(\left| \frac{1}{G} \right| \right) + \sum G_o \right]$$

which over counts the lowest order contribution (shown in fig. 2.5) to Ω of eq.(2.5), and then in the last term of eq.(2.15) we subtract off the over counted diagram. This process can be extended to the summation of all diagrams of a particular order in self-energy and not only of a particular class, which were shown in fig.(2.3). However, for the general case the counting and combinatorics becomes exceedingly complex. It is at this point that the Yang-Lee-Luttinger-Ward argument brings the result

for the most general case into focus. These authors have argued that the exact grand potential Ω , may be written in general as ⁽¹⁰⁾

$$\Omega = -\frac{V}{\beta} \text{Tr} \left[\ln \left(\frac{1}{1G} \right) + \Sigma G \right] + \Omega'(G) \quad (2.16)$$

The structure of eq.(2.16) is very similar to that of eq.(2.15). In fact the origin of all the terms, in the two equations, is quite similar. The $\Omega'(G)$ represents the sum of all those diagrams in the series for Ω in which originally only unperturbed Green's functions are used but then these unperturbed Green's functions are replaced everywhere by perturbed or exact Green's functions. Thus, $\Omega'(G)$ can be regarded as a functional of Σ whose purpose is to subtract off a series of overcounted diagrams arising from the first two terms of eq.(2.16).

Luttenger and Ward ⁽¹⁰⁾ have derived several important properties of Ω , using the expression of eq. (2.16), among which the most important is its property of stationarity with respect to first order variations in the self-energy Σ , i.e. $\frac{\delta \Omega}{\delta \Sigma} = 0$. This property of stationarity allows some approximate calculations to be done in a very elegant way as we shall see in the following.

For the interacting system of electrons and phonons we can write the equivalent of eq. (2.16) for the thermodynamic potential Ω_{el-ph} for a unit volume,

$$\begin{aligned}
\Omega_{\text{el-ph}} = & -\frac{1}{\beta} \sum_n \text{Tr} \left\{ \ln \left(\frac{1}{|G(\omega_n)|} \right) + \sum(\omega_n) G(\omega_n) \right\} \\
& + \frac{1}{2\beta} \sum_n \text{Tr} \left\{ \ln \left(\frac{1}{|D(\omega_n)|} \right) + \Pi(\omega_n) D(\omega_n) \right\} \\
& + \Omega'(G, D)
\end{aligned}
\tag{2.17}$$

where $\Pi(\omega_n)$ is phonon self-energy and $D(\omega_n)$ is the exact phonon Green's function; all other quantities are as defined above.

In writing eq.(2.16) we have omitted electron-electron Coulomb interactions, because as shown by Rice⁽¹⁷⁾ this interaction gives rise to little or no renormalization. However, screening effects can be taken into account by using screened electron-phonon coupling constants.

In analysing eq.(2.17) we first note that the phonon contribution to the oscillatory part of the thermodynamic potential is negligible. This is due to the weak coupling between the density fluctuations and the magnetic field⁽⁴⁾. The phonon self-energy $\Pi(\omega_n)$ is also independent of magnetic field, except for a small oscillatory part coming from the excitations of electrons near the Fermi surface, this too is quite negligible⁽⁵⁾. This means that the major contribution to the oscillatory part of the thermodynamic potential comes from electronic states only. Thus we can write

$$\Omega_{\text{el}} = -\frac{1}{\beta} \sum_n \text{Tr} \left\{ \ln \left(\frac{1}{|G(\omega_n)|} \right) + \sum(\omega_n) G(\omega_n) \right\} + \Omega'(G) \tag{2.18}$$

To isolate the oscillatory part of Ω , we note that the self-energy $\sum(\omega_n)$ can be decomposed into an oscillatory and a non-

oscillatory part

$$\Sigma(\omega_n) = \Sigma_{\text{nosc}}(\omega_n) + \Sigma_{\text{osc}}(\omega_n) \quad (2.19)$$

where $\Sigma_{\text{nosc}}(\omega_n)$ is that part of the self-energy which has no dHvA oscillations in it and $\Sigma_{\text{osc}}(\omega_n)$ is the oscillatory part. If we now use the stationary property of the thermodynamic potential Ω to expand it around $\Sigma_{\text{nosc}}(\omega_n)$, we get

$$\begin{aligned} \Omega = \Omega_{\text{el}} = & -\frac{1}{\beta} \sum_n \text{Tr} \left\{ \ln \left(\xi + \Sigma_{\text{nosc}}(\omega_n) - i\omega_n \right) + \right. \\ & G \left(\Sigma_{\text{nosc}}(\omega_n) \right) \Sigma_{\text{nosc}}(\omega_n) \left. \right\} + \\ & \Omega' \left\{ \Sigma_{\text{nosc}}(\omega_n) \right\} + O \left\{ \Sigma_{\text{osc}}(\omega_n) \right\}^2 \end{aligned} \quad (2.20)$$

where due to the stationary property, $\frac{\delta \Omega}{\delta \Sigma} = 0$, there is no first order term. Engelsberg and Simpson⁽⁴⁾ have estimated the last term in eq.(2.20) using an Einstein model and found it to be smaller by a factor $(\omega_c/\mu)^{1/2}$ than the leading term, so we can drop the last term in eq.(2.20). We can also drop the magnetic field dependence of the self-energy because, as can be shown, for a constant coupling Einstein model the non-oscillatory part of the self-energy has no field dependence at all⁽⁴⁾; and due to the screened interaction between electrons and phonons, any other model will not differ very significantly from the Einstein model. Writing for the magnetic field independent non-oscillatory part of the self-energy, we have¹

1. We can calculate the self-energy using Bloch states or free electron states. This, of course, introduces some "false" quantum numbers, i.e.

k_x, k_y , which necessitates taking some orbital average. We shall discuss this point further on in the work.

$$\begin{aligned}
\Omega = & -\frac{1}{\beta} \sum_n \text{Tr} \left\{ \ln \left(\xi + \Sigma_o(\omega_n) - i\omega_n \right) + \Sigma_o(\omega_n) G_1(\Sigma_o(\omega_n)) \right\} \\
& + \Omega' \{ \Sigma_o(\omega_n) \}
\end{aligned}
\tag{2.21}$$

Since our primary interest is in the dHvA oscillations, we can now use Luttinger's argument to separate the oscillatory part of Ω . Luttinger⁽⁹⁾ has shown that the oscillatory_{part} of $\Omega' \{ \Sigma_o(\omega_n) \}$ is, to an adequate approximation, equal to the negative of the second term in eq. (2.21). The basis of the argument is the non-analytical character of the Green's function which is responsible for the dHvA oscillations. We can finally write

$$\begin{aligned}
\Omega_{osc} = & -\frac{1}{\beta} \text{Tr} \sum_n \ln \left(\left| \frac{1}{G_1(\omega_n)} \right| \right) \\
= & -\frac{1}{\beta} \text{Tr} \sum_n \ln \left(\xi + \Sigma_o(i\omega_n) - i\omega_n \right)
\end{aligned}
\tag{2.22}$$

where we have written $\Sigma_o(i\omega_n)$ in place of $\Sigma_o(\omega_n)$ to point out explicitly that it is the finite temperature self-energy evaluated on the imaginary energy axis.

As is mentioned in the footnote on the previous page $\Sigma_o(i\omega_n)$ is actually $\Sigma_o(k_z, k_\perp, i\omega_n)$ where k_z is the wave vector in the direction of the magnetic field and k_\perp is the wave vector transverse to the magnetic field, over which some suitable average will be defined⁽¹³⁾. In the following derivation depending on convenience, we will exhibit or suppress the various dependences of the self-energy as well as the energy ξ .

2.2 Basic formula for de Haas-van Alphen Effect

Our objective now is to develop from eq.(2.22) a formula that describes the dHvA oscillations in an interacting system. To begin with we use the effective mass approximation for the band structure, which is good for some metals at least near the Fermi surface. We can then write the non-interacting single particle spectrum (Landau levels) as

$$\epsilon_{k_z, l, \sigma} = \frac{k_z^2}{2m} + \left(l + \frac{1}{2}\right) \omega_c + \sigma g \mu_B B - \mu \quad (2.23)$$

where,

$\omega_c = (eB/mc)$ the cyclotron frequency,

B = the magnetic field in the z-direction,

μ_B = the Bohr magneton, $\left(\mu_B \equiv \frac{e\hbar}{2mc}\right)$

$\sigma = \pm 1/2$, are the spin quantum numbers of the electron,

g = the electron band g factor, and

μ = the chemical potential,

m = the band mass of the electron, and l is the quantum number for the cyclotron motion of the electron.

If we treat the logarithm of eq.(2.22) as a distribution we can apply the following integral representations:

$$\begin{aligned} \text{when } \operatorname{Im} \{ i\omega_n - \Sigma(i\omega_n) \} > 0 ; \\ \ln [\epsilon - i\omega_n + \Sigma(i\omega_n)] = \lim_{b \rightarrow 0^+} \int_b^{b+i\delta} \frac{ds}{s} e^{-s[\epsilon - i\omega_n + \Sigma(i\omega_n)]} \end{aligned} \quad (2.24)$$

$$\begin{aligned} \text{and, when } \operatorname{Im} \{ i\omega_n - \Sigma(i\omega_n) \} < 0 ; \\ \ln [\epsilon - i\omega_n + \Sigma(i\omega_n)] = \lim_{b \rightarrow 0^+} \int_{b-i\delta}^b \frac{ds}{s} e^{-s[\epsilon - i\omega_n + \Sigma(i\omega_n)]} \end{aligned} \quad (2.25)$$

Now, from the spectral representation of the self-energy function

$$\Sigma(i\omega_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\Gamma(\omega)}{i\omega_n - \omega} d\omega \quad ; \quad \Gamma(\omega) \geq 0 \quad (2.26)$$

we note that,

$$\text{Im } \Sigma(i\omega_n) = -\frac{\omega_n}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega \Gamma(\omega)}{\omega_n^2 + \omega^2} \quad (2.27)$$

so, $\text{Im } \Sigma(i\omega_n) < 0$ when $\omega_n > 0$;

and $\text{Im } \Sigma(i\omega_n) > 0$ when $\omega_n < 0$.

Thus we can write Ω as a sum of contributions from $\omega_n > 0$ and from $\omega_n < 0$, which we call Ω_+ and Ω_- respectively, where

$$\Omega = (\Omega_+) + (\Omega_-)$$

and

$$\Omega_+ = -\frac{1}{\beta} \text{Tr} \sum_n \lim_{b \rightarrow 0^+} \int_b^{b+i\infty} \frac{ds}{s} e^{-s[\epsilon(k_z, l, \sigma) - i\omega_n + \Sigma(k_z, i\omega_n)]} \quad (2.28)$$

$$\Omega_- = -\frac{1}{\beta} \text{Tr} \sum_n \lim_{b \rightarrow 0^+} \int_{b-i\infty}^b \frac{ds}{s} e^{-s[\epsilon(k_z, l, \sigma) - i\omega_n + \Sigma(k_z, i\omega_n)]} \quad (2.29)$$

Before we proceed further, we may verify that the above relations does indeed give the familiar result for free electrons i.e. for

$\Sigma(k_z, i\omega_n) = 0$. Noting that $\text{Re } s > 0$; we have the following results

$$\int_{-\infty}^{\infty} dk_z e^{-\frac{s k_z^2}{2m}} = \left(\frac{2m}{s}\right)^{1/2}$$

$$\sum_{l=0}^{\infty} e^{-s \omega_c (l+1/2)} = \frac{1}{2 \sinh\left(\frac{s \omega_c}{2}\right)}$$

More over for $\omega_n > 0$, $\text{Im } s > 0$;

$$\sum_{n=0}^{\infty} e^{is(2n+1)\pi/\beta} = \frac{1}{2i \sin(s\pi/\beta)}$$

and for $\omega_n < 0$, $\text{Im } s < 0$,

$$\sum_{n=0}^{\infty} e^{-is(2n+1)\pi/\beta} = \frac{1}{2i \sin(s\pi/\beta)}$$

With these sums and integrals done, the two integrals may now be combined to give

$$\Omega = \frac{m \omega_c}{(2\pi)^{3/2}} \left(\frac{2m}{2\pi i}\right)^{1/2} \int_{b-i\infty}^{b+i\infty} \frac{e^{s\mu} \pi \csc(\pi s/\beta) \cdot 2 \cosh\left(\frac{1}{2} g \mu_B \cdot B \cdot s\right)}{s^{3/2} \sinh\left(\frac{s \omega_c}{2}\right)} ds$$

(2.30)

from which the oscillatory behaviour can be extracted by applying the residue theorem at the poles along the imaginary s -axis at $s = \frac{(2n+1)\pi i}{\omega_c}$ where $n = \pm 1, \pm 2, \pm 3, \dots$.

In the more general case (which is of interest here) when $\sum (k_z, i\omega_n) \neq 0$ the evaluation of the oscillatory part is still straight-forward. First

the sum over Landau levels and spin gives

$$\Omega_+ = -\frac{1}{\beta} \frac{m\omega_c}{2\pi^2} \sum_n \int_{-\infty}^{\infty} dk_z \int_b^{b+i\omega} \frac{ds}{s} e^{-s \left[\frac{k_z^2}{2m} - \mu - i\omega_n + \sum (k_z, i\omega_n) \right]} \times$$

$$\left\{ \cosh\left(\frac{1}{2} g \mu_B B s\right) / \sinh\left(\frac{s\omega_c}{2}\right) \right\}$$

(2.31a)

and

$$\Omega_- = \frac{1}{\beta} \frac{m\omega_c}{2\pi^2} \sum_n \int_{-\infty}^{\infty} dk_z \int_{b-i\omega}^b \frac{ds}{s} e^{-s \left[\frac{k_z^2}{2m} - \mu - i\omega_n + \sum (k_z, i\omega_n) \right]} \times$$

$$\left\{ \cosh\left(\frac{1}{2} g \mu_B B s\right) / \sinh\left(\frac{s\omega_c}{2}\right) \right\} \quad (2.31b)$$

The k_z integration may also be done at this stage by, say, the method of stationary phase; but it is not necessary for obtaining an extension of the Fowler-Prange theorem, in which we would be interested.

Once again, the oscillatory contribution arises from the poles introduced by the sum over Landau levels, which are located on the imaginary s -axis at $s = \frac{2\pi i r}{\omega_c}$, $r = \pm 1, \pm 2, \dots$. If we deform the contours of Ω_+ and Ω_- to encircle the poles in the upper half of the s -plane and the poles in the lower half of the s -plane respectively; we have from the sum of the residues at these poles-

$$\Omega_+ = -\frac{m\omega_c}{\pi^2 \beta} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk_z \sum_{r=1}^{\infty} \frac{(-1)^r}{r} e^{-\frac{2\pi i r}{\omega_c} \left[\frac{k_z^2}{2m} - \mu - i\omega_n + \sum (k_z, i\omega_n) \right]}$$

$$\times \cos\left(\frac{g \mu_B \pi r B}{\omega_c}\right)$$

(2.32a)

and

$$\Omega_- = -\frac{m\omega_c}{\pi^2\beta} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk_z \sum_{r=1}^{\infty} \frac{(-1)^r}{r} e^{-\frac{2\pi r}{\omega_c} \left[\frac{k_z^2}{2m} - \mu + \Sigma(k_z, i\omega_n) \right]} \times \cos\left(\frac{g\mu_B\pi r B}{\omega_c}\right) \quad (2.32b)$$

Finally, we combine the two parts to give

$$\Omega = -\frac{2m\omega_c}{\pi^2\beta} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk_z \sum_{r=1}^{\infty} \frac{(-1)^r}{r} \cos\frac{2\pi r}{\omega_c} \left[\frac{k_z^2}{2m} - \mu + \text{Re}\Sigma(k_z, i\omega_n) \right] \times e^{-\frac{2\pi r}{\omega_c} \left[\omega_n - \text{Im}\Sigma(k_z, i\omega_n) \right]} \cos\left(\frac{g\mu_B\pi r B}{\omega_c}\right) \quad (2.33)$$

Except for the remaining k_z integration, the above equation may be recognized as the well known Fowler-Prange theorem. The above derivation shows with clarity, how the dHvA oscillations of the magnetic susceptibility separates the real and imaginary parts of the self-energy, when evaluated on the imaginary energy axis.

Our aim now is to extend the Fowler and Prange's high temperature result, to a region including lower temperatures by carrying out an approximate sum over n . Since we are primarily interested in the amplitude we ignore the real part of the self-energy $\Sigma(k_z, i\omega_n)$ which appears in the frequency. With this simplification, it becomes convenient to do the k_z integration by, say, the method of stationary phase to give

$$\Omega = -2 \frac{(m\omega_c)^{3/2}}{\pi^2\beta} \sum_{n=0}^{\infty} \sum_{r=1}^{\infty} \frac{(-1)^r}{r} \cos\left(\frac{2\pi r}{\omega_c} \pm \pi/4\right) e^{-\frac{2\pi r}{\omega_c} \left[\omega_n - \text{Im}\Sigma(0, i\omega_n) \right]} \times \cos\left(\frac{\pi g\mu_B r B}{\omega_c}\right) \quad (2.34)$$

where k_z (the quantum number of the orbit) is zero in this case.

Now, rather than using the customary method⁽¹⁰⁾ for doing the sum, we use the Poisson sum formula

$$\sum_{n=0}^{\infty} f\left[\frac{(2n+1)\pi i}{\beta}\right] = \sum_{\nu=-\infty}^{\infty} \int_0^{\infty} dy f\left[\frac{(2y+1)\pi i}{\beta}\right] e^{-2\pi i \nu y} \quad (2.35)$$

If we expand $\text{Im} \sum (2y+1)\frac{\pi i}{\beta}$ around $y = 0$, and retain only the linear term; we have

$$\begin{aligned} \text{Im} \sum (2y+1)\frac{\pi i}{\beta} &= \text{Im} \sum \left(\frac{\pi i}{\beta}\right) + y \frac{\partial}{\partial y} \text{Im} \sum (2y+1)\frac{\pi i}{\beta} \Big|_{y=0} \\ &= \text{Im} \sum (i\omega_0) + \frac{2\pi y}{\beta} \frac{\partial}{\partial \omega_0} [\text{Im} \sum (i\omega_0)] \end{aligned} \quad (2.36)$$

where $\omega_0 = \pi/\beta$. The dHvA amplitude becomes then

$$\begin{aligned} \sum_{\nu=-\infty}^{\infty} e^{-\frac{2\pi \tau}{\omega_c} [\omega_0 - \text{Im} \sum (i\omega_0)]} \times \int_0^{\infty} dy e^{-2\pi i \nu y} \times \\ \left\{ e^{-\frac{4\pi \tau \omega_0}{\omega_c} y} \left[1 - \frac{\partial}{\partial \omega_0} \text{Im} \sum (i\omega_0) \right] \right\} \end{aligned} \quad (2.37)$$

Performing the now trivial y -integration yields for the amplitude

$$e^{-\frac{2\pi \tau}{\omega_c} [\omega_0 - \text{Im} \sum (i\omega_0)]} \sum_{\nu=-\infty}^{\infty} \left\{ 2\pi i \nu + \frac{4\pi \tau \omega_0}{\omega_c} \left[1 - \frac{\partial}{\partial \omega_0} \text{Im} \sum (i\omega_0) \right] \right\}^{-1} \quad (2.38)$$

The infinite sum over ν is just a Mittag-Leffler expansion of

$$\frac{1}{1 - e^{-\frac{4\pi r \omega_0}{\omega_c} \left\{ 1 - \frac{\partial}{\partial \omega_0} \text{Im} \Sigma(i\omega_0) \right\}}}$$
(2.39)

Thus, to this approximation, the amplitude finally takes the form

$$\frac{e^{-\frac{2\pi r}{\omega_c} [\omega_0 - \text{Im} \Sigma(i\omega_0)]}}{1 - e^{-\frac{4\pi r}{\omega_c} \omega_0 \left[1 - \frac{\partial}{\partial \omega_0} \text{Im} \Sigma(i\omega_0) \right]}}$$
(2.40)

and the oscillatory part of the thermodynamic potential is

$$\Omega = \frac{-2(m\omega_c)^{3/2}}{\pi^2 \beta} \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \cos\left(\frac{2\pi r \mu}{\omega_c} \pm \frac{\pi}{4}\right) \times$$

$$\cos\left(\frac{\pi g \mu_B r B}{\omega_c}\right) \left\{ \frac{e^{-\frac{2\pi r}{\omega_c} [\omega_0 - \text{Im} \Sigma(i\omega_0)]}}{1 - e^{-\frac{4\pi r}{\omega_c} \omega_0 \left[1 - \frac{\partial}{\partial \omega_0} \text{Im} \Sigma(i\omega_0) \right]}} \right\}$$
(2.41)

As an application of the above formula to see how various interactions contribute to amplitude effects, we now consider two specific cases (1) the self-energy due to phonon scattering in a pure system and (2) the self-energy due to fixed impurity scattering. Later in chapter III, we will derive the expressions for phonon scattering in an impure (substitutional binary) alloy as well.

(1) The electron-phonon self-energy : The electron-phonon self-energy in a pure metal, when evaluated at the first pole of the Fermi function (from eq. 4.32 of ch. IV) is

$$\Sigma(k_z=0, \omega_0) = -\omega_0 \lambda i \quad (2.42)$$

where λ is the enhancement factor. Further more

$$\frac{\partial}{\partial \omega_0} \text{Im} \Sigma(k_z=0, \omega_0) = -\lambda \quad (2.43)$$

to order of magnitude considered.

(2) Fixed impurity scattering : Any self-energy in general can be written in terms of its spectral representation as⁽²⁾

$$\Sigma(\vec{k}, \omega_n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\Gamma(\vec{k}, \omega)}{i\omega_n - (\omega - \mu)} d\omega \quad (2.44)$$

where $\Gamma(\vec{k}, \omega)$ is the self-energy spectral function, and

$$\Gamma(\vec{k}, \omega) = -2 \text{Im} \Sigma(\vec{k}, \omega) \geq 0 \quad (2.45)$$

where ω is always on the real energy axis. $\Gamma(\vec{k}, \omega)$ is in fact the discontinuity in the self-energy $\Sigma(\vec{k}, \omega)$ across the cut on the real energy axis. In the case of randomly placed uncorrelated scattering potentials, the spectral function may be expressed in terms of the scattering t-matrix as⁽²⁾

$$\Gamma(\vec{k}, \omega) = 2\pi N_i \sum_{\vec{q}} |t_{\vec{k}, \vec{q}}|^2 \delta(\omega - \epsilon_{\vec{q}}) \quad (2.46)$$

which is essentially the optical theorem.

Now for the purpose of our formulation, we require the dlivA orbital average of

$$\text{Im } \Sigma(k_z=0, \omega_0) = -\frac{\omega_0}{2\pi} \int_{-\infty}^{\infty} \frac{\Gamma(\omega)}{\omega_0^2 + (\omega - \mu)^2} d\omega \quad (2.47)$$

as well as of

$$\begin{aligned} \frac{\partial}{\partial \omega_0} \text{Im } \Sigma(k_z=0, \omega_0) = & -\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\Gamma(\omega) d\omega}{\omega_0^2 + (\omega - \mu)^2} \\ & + 2\omega_0^2 \int_{-\infty}^{\infty} \frac{\Gamma(\omega) d\omega}{[\omega_0^2 + (\omega - \mu)^2]^2} \end{aligned} \quad (2.48)$$

Examining eq.(2.47) and the first term of eq.(2.48), we shall take the customary low temperature limit used in treating impurity scattering. Then as $T \rightarrow 0$, we have

$$\lim_{\omega_0 \rightarrow 0} \frac{\omega_0}{\omega_0^2 + (\omega - \mu)^2} = \pi \delta(\omega - \mu) \quad (2.49)$$

$$\text{so that, } \text{Im } \Sigma(k_z=0, \omega_0 \rightarrow 0) = -\frac{\Gamma(\mu)}{2} \quad (2.50)$$

$$\text{and } \frac{\partial}{\partial \omega_0} \text{Im } \Sigma(k_z=0, \omega_0 \rightarrow 0) = -\frac{\Gamma(\mu)}{2\omega_0} \quad (2.51)$$

where, we have ignored the second term of eq. (2.48). If we assume that the self-energy due to static impurity is temperature independent, then the only contribution comes from eq.(2.50). In this case we have for the contribution to the amplitude from static impurity scattering as

$$A_r^{\text{st. imp}} \sim e^{-\frac{2\pi\tau}{\omega_c} |\text{Im} \Sigma(\mu)|} \sim e^{-\frac{2\pi\tau}{\omega_c} \frac{\Gamma(\mu)}{2}} \quad (2.52)$$

Comparing this with the expression defining the Dingle temperature T_D i.e. $e^{-\frac{2\pi^2\tau k_B T_D}{\omega_c}}$, we see that

$$T_D = \frac{\Gamma(\mu)}{2\pi k_B} \quad (2.53)$$

This then is the finite temperature derivation of Dingle temperature.

Including both impurity and phonon scattering, we can write for the amplitude of the r -th harmonic of the dHvA oscillations as

$$A_r \approx \frac{e^{-\frac{2\pi\tau}{\omega_c} \frac{\Gamma(\mu)}{2}} e^{-\frac{2\pi\tau}{\omega_c} \omega_0 \frac{m^*}{m}}}{1 - e^{-\frac{4\pi\tau}{\omega_c} \omega_0 \left[\frac{m^*}{m} + \frac{\Gamma(\mu)}{2\omega_0} \right]}} \approx \frac{1}{\sinh \frac{2\pi\tau}{\omega_c} \left[\frac{\Gamma(\mu)}{2} + \omega_0 \frac{m^*}{m} \right]} \quad (2.54)$$

where we have used the relation $\lambda = \left(\frac{m^*}{m} - 1 \right)$. m^* is called the el-ph enhanced mass.

III. ELECTRON-PHONON INTERACTION IN DILUTE ALLOYS.

As noted in the previous chapter, to calculate the thermodynamic potential for an interacting system, we need to know the electron self-energy of interaction on the imaginary energy axis. Then we can use eq. (2.41) to calculate the amplitude of the oscillations.

A formal calculation of the electron-phonon self-energy in a dilute substitutional binary alloy has been done by Hicks⁽⁷⁾. In Hicks calculation modification of ionic force constants was ignored. Although there are obviously cases for which this effect is important, no attempt to include the effect has been made in the present work. In the following we give a brief outline of the procedure used and then in chapter IV go on to calculate the self-energy contributions which are of relevance in our case.

The starting point in the calculation is to write the full Hamiltonian of the alloy as

$$\begin{aligned}
 H = & \sum_i \frac{p_i^2}{2m} + \sum_{i,\alpha} V_\alpha(\vec{r}_i - \vec{R}_\alpha) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \\
 & + \sum_\alpha \frac{P_\alpha^2}{2M} + \frac{1}{2} \sum_{\alpha \neq \beta} V(\vec{R}_\alpha - \vec{R}_\beta) + \sum_\lambda \frac{P_\lambda^2}{2\epsilon}
 \end{aligned}
 \tag{3.1}$$

here,

i and j sum over electron co-ordinates \vec{r}_i and \vec{r}_j ,

α and β sum over all ion co-ordinates \vec{R}_α and \vec{R}_β ,

λ sums over impurity co-ordinates,

V_α is electron-ion interaction on the α -th site,

m is electron mass,

M is host ion mass, and

M' is impurity ion mass,

$$\frac{1}{\epsilon} = \frac{1}{M'} - \frac{1}{M} \quad ; \text{ and} \quad (3.2)$$

p_i and P_α denote the momenta of the i -th electron and α -th ion respectively.

It is possible to separate the above Hamiltonian into two parts H_{ph} and H_{el} corresponding to phonons and electrons respectively using an extension of the Born-Oppenheimer theorem to the case of continuum electron states⁽¹⁸⁾. We have

$$H_{ph} = \sum_{\alpha} \frac{P_{\alpha}^2}{2M} + \frac{1}{2} \sum_{\alpha \neq \beta} V(\vec{R}_{\alpha} - \vec{R}_{\beta}) + \sum_{\alpha \neq \beta} E_k(\vec{R}_{\alpha} - \vec{R}_{\beta}) + \sum_{\lambda} \frac{P_{\lambda}^2}{2\epsilon} \quad (3.3)$$

$$H_{el} = \sum_i \frac{p_i^2}{2m} + \sum_{i, \alpha} V_{\alpha}(\vec{r}_i - \vec{R}_{\alpha}) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \quad (3.4)$$

The term $\sum_{\alpha \neq \beta} E_k(\vec{R}_{\alpha} - \vec{R}_{\beta})$ represents electronic energies for fixed ion separation $(\vec{R}_{\alpha} - \vec{R}_{\beta})$. Though in general this correction depends on the individual electronic states (as indicated by the suffix \vec{k}), it is slowly varying in \vec{k} for the electronic states near the Fermi surface⁽¹⁸⁾. Therefore dropping the subscript \vec{k} and absorbing the energy E into V by writing it as V_{eff} , we get

$$H_{ph} = \sum_{\alpha} \frac{P_{\alpha}^2}{2M} + \frac{1}{2} \sum_{\alpha \neq \beta} V_{eff}(\vec{R}_{\alpha} - \vec{R}_{\beta}) + \sum_{\lambda} \frac{P_{\lambda}^2}{2\epsilon} \quad (3.5)$$

For states that show binding V_{eff} has the shape typical of bound molecular states. Assuming then that the displacement of the α -th ion, from its equilibrium position of minimum energy, $\delta \vec{R}_{\alpha_0}$ is small, we can expand V_{eff} about its equilibrium position \vec{R}_{α_0} and get

$$H_{ph} = \sum_{\alpha} \frac{P_{\alpha}^2}{2M} + \frac{1}{2} \sum_{\alpha \neq \beta} \Lambda_{\alpha, \beta}^{\alpha, \beta} \delta R_{\alpha} \delta R_{\beta} + \sum_{\lambda} \frac{P_{\lambda}^2}{2\epsilon} \quad (3.6)$$

where α and β sum over the three possible vector directions.

$$\Lambda_{\alpha, \beta}^{\alpha, \beta} = \left. \frac{\partial^2 V_{eff}(\vec{R}_{\alpha} - \vec{R}_{\beta})}{\partial R_{\alpha} \partial R_{\beta}} \right|_{\substack{\vec{R}_{\alpha} = \vec{R}_{\alpha_0} \\ \vec{R}_{\beta} = \vec{R}_{\beta_0}}} \quad (3.7)$$

and,

$$\Lambda_{\alpha, \alpha}^{\alpha, \alpha} = \sum_{\substack{\beta \\ \beta \neq \alpha}} \left. \frac{\partial^2 V_{eff}(\vec{R}_{\alpha} - \vec{R}_{\beta})}{\partial R_{\alpha}^2} \right|_{\substack{\vec{R}_{\alpha} = \vec{R}_{\alpha_0} \\ \vec{R}_{\beta} = \vec{R}_{\beta_0}}} \quad (3.8)$$

Now defining Matsubara Green's function as

$$D_{st}^{\alpha, \beta}(\tau) = -\langle T_{\tau} \delta R_{s\alpha}(\tau) \delta R_{t\beta}(0) \rangle \quad (3.9)$$

where $\delta R_{s\alpha}(\tau)$ is the ionic displacement operator as expressed in the Heisenberg picture in which ixt (t = real time) has been analytically continued to $(1/k_B T) = \tau$; and T_{τ} is the imaginary time-temperature ordering operator. The bracket $\langle \dots \rangle$ represents a thermodynamic grand canonical ensemble average.

With the definition of eq.(3.9) for the phonon Green's function and with the Hamiltonian of eq.(3.6) it is possible to generate a hierarchy of equations of motion and an iterative process which will permit its (i.e. $D_{s,t}^{\alpha, \beta}(\tau)$) determination to some order in the coupling constants. When this is done it is easy to get the phonon Green's function for the

disordered mass substitutional lattice. However, for the purpose of separating the various contributions to view them eventually as corrections to the normal host system⁽⁸⁾, it is convenient to obtain three different types of ensemble averaged Green's functions which correspond to correlations of host and impurity atoms amongst themselves and with each other. Thus one has

1. For host-host correlations

$$\langle D_s(\vec{q}|\omega_n) \rangle = d_s(\vec{q}|\omega_n) \frac{\left\{ 1 + \frac{M}{\epsilon} c - (1-c) \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} M \omega_s^2(\vec{q}') d_s(\vec{q}'|\omega_n) \right\}}{1 - f_s(\vec{q}, \omega_n)} \quad (3.10)$$

2. For impurity-impurity correlations

$$\langle D_s^{d-d}(\vec{q}|\omega_n) \rangle = \frac{M}{M'} \frac{d_{st}(\vec{q}|\omega_n)}{(1 - f_s(\vec{q}|\omega_n))} \left\{ 1 - M \omega_s^2(\vec{q}) \frac{M}{\epsilon} (1-c) \frac{1}{N} \sum_{\vec{q}'} d_s(\vec{q}'|\omega_n) \right\} \quad (3.11)$$

3. For host and impurity correlations

$$\langle D_s^d(\vec{q}|\omega_n) \rangle = \frac{M}{M'} \frac{d_{st}(\vec{q}|\omega_n)}{1 - f_s(\vec{q}|\omega_n)} \quad (3.12)$$

where,
$$d_s(\vec{q}|\omega_n) = \frac{1}{M} \frac{1}{\omega_n^2 - \omega_s^2(\vec{q})} ; \quad \omega_n = \frac{2n\pi i}{\beta}$$

$$f_s(\vec{q}|\omega_n) = \frac{M}{\epsilon} c M \omega_s^2(\vec{q}) d_s(\vec{q}|\omega_n) + \left\{ (1-c) \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} M \omega_s^2(\vec{q}') d_s(\vec{q}'|\omega_n) \right\} \quad (3.13)$$

and concentration $c = N_i / N$; where, N is the number of host atoms in a unit volume and N_i is the number of impurity atoms in a unit volume. We assume that ^{the} concentration c is low so that $N \gg N_i$.

After getting these phonon Green's functions for the impure lattice one has to consider some process of coupling these with the electron Green's function. In coupling the electrons to the phonons, according to the famous and important theorem of Migdal⁽¹⁵⁾, all vertex corrections to the interaction may be ignored as they contribute to order $(m/M)^{1/2}$ i.e. square root of electron to ion mass ratio, compared to the lowest order term. So the principal contribution to the electron-phonon self-energy comes from the term with the Feynman diagram as shown in fig. (3.1).



Fig. 3.1

There are then three different contributions to the electron self-energy which arises from the correlation of host and impurity sites in the lattice. These to order linear in concentration c (per unit volume) are

1.

$$\begin{aligned} \Sigma_a(\vec{k}|\omega_n) = & -C \sum_{s, \vec{q}, \vec{R}_i} \frac{1}{P} \sum_{\omega_{n'}} G_0(\vec{R}_i|\omega_{n'}) D_s^{d-d}(\vec{q}|\omega_n - \omega_{n'}) \\ & \times \Delta^2(\vec{k} - \vec{R}_i) [(\vec{k} - \vec{R}_i) \cdot \hat{\epsilon}_s]^2 \end{aligned} \quad (3.14)$$

2.

$$\sum_b(\vec{k}|\omega_n) = -Nc \sum_{s, \vec{q}} \frac{1}{\beta} \sum_{\omega_n'} G_o(\vec{k}-\vec{q}|\omega_n') D_s^d(\vec{q}|\omega_n-\omega_n') \times$$

$$\left\{ V(\vec{q}) \Delta(-\vec{q}) + V(-\vec{q}) \Delta(\vec{q}) \right\} (\vec{q} \cdot \hat{\epsilon}_s)^2$$

(3.15)

3.

$$\sum_c(\vec{k}|\omega_n) = -N \sum_{s, \vec{k}_1, \vec{q}} \frac{1}{\beta} \sum_{\omega_n'} G_o(\vec{k}_1|\omega_n') D_s(\vec{q}|\omega_n-\omega_n') \times$$

$$\vec{q} = \vec{k} - \vec{k}_1 + \vec{q} \quad \left[V(\vec{k} - \vec{k}_1) \right]^2 \left[(\vec{k} - \vec{k}_1) \cdot \hat{\epsilon}_s \right]^2$$

(3.16)

where the diagonality in \vec{k} arises from the uncorrelated ensemble averages over the impurity sites, and Δ is the Fourier component of the difference in the scattering potential at the impurity site; and

$$V(\vec{k}) = \frac{1}{\sqrt{\text{vol}}} \int d\vec{r} V(\vec{r}) e^{i\vec{k} \cdot \vec{r}} = \int d\vec{r} V(\vec{r}) e^{i\vec{k} \cdot \vec{r}}$$

(3.17)

for a unit volume.

In the next chapter several approximations are made and these three contributions are evaluated for points on the imaginary energy axis. Infact, as the formulation in the previous chapter indicates, evaluation at the point $\omega_o = \frac{\pi i}{\beta}$ is all that is important.

IV. ELECTRON-PHONON SELF-ENERGY ON THE IMAGINARY ENERGY AXIS FOR A DILUTE ALLOY.

From chapter III we have the formal expressions, eqs. (3.14), (3.15) and (3.16), for the various contributions to the electron-phonon self-energy in a dilute alloy.

Rewriting eq. (3.14), we have

$$\sum_a(\vec{k}|\omega_n) = -C \sum_{s, \vec{q}, \vec{k}_1} \frac{1}{\beta} \sum_{\omega_{n'}} G_0(\vec{k}_1|\omega_{n'}) D_s^{d-d}(\vec{q}|\omega_n - \omega_{n'}) \times \Delta^2(\vec{k} - \vec{k}_1) [(\vec{k} - \vec{k}_1) \cdot \vec{\epsilon}_s]^2 \quad (3.14)$$

For convenience we denote, $S_a(\vec{k}_1|\vec{q}) = \sum_{\omega_{n'}} G_0(\vec{k}_1|\omega_{n'}) D_s^{d-d}(\vec{q}|\omega_n - \omega_{n'})$

Then substituting for $D_s^{d-d}(\vec{q}|\omega_n - \omega_{n'})$ from eq. (3.11) and using for the electron Green's function $G_0(\vec{k}_1|\omega_{n'}) = \frac{1}{\omega_{n'} - \tilde{\epsilon}_{\vec{k}_1}}$, where $\tilde{\epsilon}_{\vec{k}_1} = (\epsilon_{\vec{k}_1} - \mu)$

we get

$$S_a(\vec{k}_1|\vec{q}) = \sum_{\omega_{n'}} \frac{1}{\omega_{n'} - \tilde{\epsilon}_{\vec{k}_1}} \cdot \frac{M}{M'} \times \left\{ \frac{d_s(\vec{q}|\omega_n - \omega_{n'}) \left(1 - \frac{M}{\epsilon} M \omega_s^2(\vec{q}) \frac{1}{N} \sum_{\vec{q}'} d_s(\vec{q}'|\omega_n - \omega_{n'}) \right)}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} M \omega_s^2(\vec{q}') d_s(\vec{q}'|\omega_n - \omega_{n'})} \right\} \quad (4.1)$$

Considering an isotropic phonon spectrum, so that $\omega_s^2(\vec{q}) = \omega^2(q)$ and

using

$$d_s(\vec{q}|\omega_n - \omega_{n'}) = \frac{1}{M} \frac{1}{(\omega_n - \omega_{n'})^2 - \omega_s^2(\vec{q})} = \frac{1}{M} \frac{1}{(\omega_n - \omega_{n'})^2 - \omega^2(q)}$$

we get

$$S_a(\vec{k}, \vec{q}) = \frac{1}{M'} \sum_{\omega_n'} \frac{1}{\omega_n' - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{(\omega_n - \omega_n')^2 - \omega^2(\vec{q})} \times$$

$$\left\{ \frac{1 - \frac{M}{\epsilon} \omega^2(\vec{q}) \frac{1}{N} \sum_{\vec{q}'} \frac{1}{(\omega_n - \omega_n')^2 - \omega^2(\vec{q}')}}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{\omega^2(\vec{q}')}{(\omega_n - \omega_n')^2 - \omega^2(\vec{q}')}} \right\} \quad (4.2)$$

The summation over \vec{q}' is easily done within a Debye model, and we find

$$S_a(\vec{k}, \vec{q}) = \frac{1}{M'} \sum_{\omega_n'} \frac{1}{\omega_n' - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{(\omega_n - \omega_n')^2 - \omega^2(\vec{q})} \times$$

$$\left\{ \frac{1 - \frac{3M}{\omega_D^3 \epsilon} \omega^2(\vec{q}) \left\{ \frac{\omega_n - \omega_n'}{2} \ln \left| \frac{\omega_n - \omega_n' + \omega_D}{\omega_n - \omega_n' - \omega_D} \right| - \omega_D \right\}}{1 + \frac{3M}{\omega_D^3 \epsilon} \left[(\omega_n - \omega_n')^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - \omega_n')^3}{2} \ln \left| \frac{\omega_n - \omega_n' - \omega_D}{\omega_n - \omega_n' + \omega_D} \right| \right]} \right\} \quad (4.3)$$

where ω_D is the Debye frequency.

Converting the ω_n' sum into a contour integral in the standard way using the Fermi function, $f(x) = \frac{1}{e^{\beta x} + 1}$, which has poles at

$$x = \frac{(2n'+1)\pi i}{\beta} \quad ; \text{ so that the sum is reproduced exactly by the}$$

integral, we have

$$S_a(\vec{k}, \vec{q}) = \frac{1}{M'} \left(-\frac{\beta}{2\pi i} \right) \int_C \frac{f(x)}{x - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{(\omega_n - x)^2 - \omega^2(\vec{q})} \times$$

$$\left\{ \frac{1 - A \omega^2(\vec{q}) \left[\frac{\omega_n - x}{2} \ln \left| \frac{\omega_n - x + \omega_D}{\omega_n - x - \omega_D} \right| - \omega_D \right]}{1 + A \left[(\omega_n - x)^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - x)^3}{2} \ln \left| \frac{\omega_n - x - \omega_D}{\omega_n - x + \omega_D} \right| \right]} \right\} \quad (4.4)$$

where $A = \frac{3M}{\omega_D^2 \epsilon}$. The contour C and the analytical structure of the integral is shown in fig.(4.1). In the complex z plane the integrand has simple poles at $\tilde{\epsilon}_{\vec{k}_1}$, $\omega_n \pm \omega(\vec{q})$ and $\omega_n \pm \omega_L$ and logarithmic branch points at $\omega_n \pm \omega_D$. Here ω_L is the frequency of the localized mode which occurs for light impurity ($\frac{M}{\epsilon}$ positive) as a pole of the phonon Green's function of the disordered lattice. If the impurity is heavy there appears a "virtual level" and in that case we can put $\omega_L = 0$ in the following derivation. Now deforming the contour outward to infinity (fig. 4.2) we pick up contributions from the poles as well as the branch points. In appendix (B) we show that the branch point contributions are negligible. Hence, omitting them from consideration, we get from Cauchy's residue theorem

$$\begin{aligned}
 S_a(\vec{k}_1, \vec{q}) = & \frac{1}{M} \left(\frac{-\beta}{2\pi i} \right) (-2\pi i) \times \\
 & \left\{ \left[\frac{f(\tilde{\epsilon}_{\vec{k}_1})}{(\omega_n - \tilde{\epsilon}_{\vec{k}_1}) - \omega^2(\vec{q})} \frac{1 - A\omega^2(\vec{q}) \left[\frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1}}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1} + \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_1} - \omega_D} \right| - \omega_D \right]}{1 + A \left[(\omega_n - \tilde{\epsilon}_{\vec{k}_1})^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - \tilde{\epsilon}_{\vec{k}_1})^3}{2} \right]} \right. \right. \\
 & \quad \left. \left. \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1} - \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_1} + \omega_D} \right| \right] \right. \\
 & + \left[\frac{f(\omega_n + \omega(\vec{q}))}{\omega_n + \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}_1}} \cdot \frac{1}{2\omega(\vec{q})} \mathcal{F}_a[\omega(\vec{q})] \right] \\
 & + \left[\frac{f(\omega_n - \omega(\vec{q}))}{\omega_n - \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}_1}} \cdot \frac{1}{-2\omega(\vec{q})} \mathcal{F}_a[\omega(\vec{q})] \right] \\
 & + \left[\frac{f(\omega_n + \omega_L)}{\omega_n + \omega_L - \tilde{\epsilon}_{\vec{k}_1}} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) \right] \\
 & + \left[\frac{f(\omega_n - \omega_L)}{\omega_n - \omega_L - \tilde{\epsilon}_{\vec{k}_1}} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \frac{\mathcal{F}_a'(\omega_L)}{(-1)} \right] \left. \right\}
 \end{aligned}$$

(4.5)

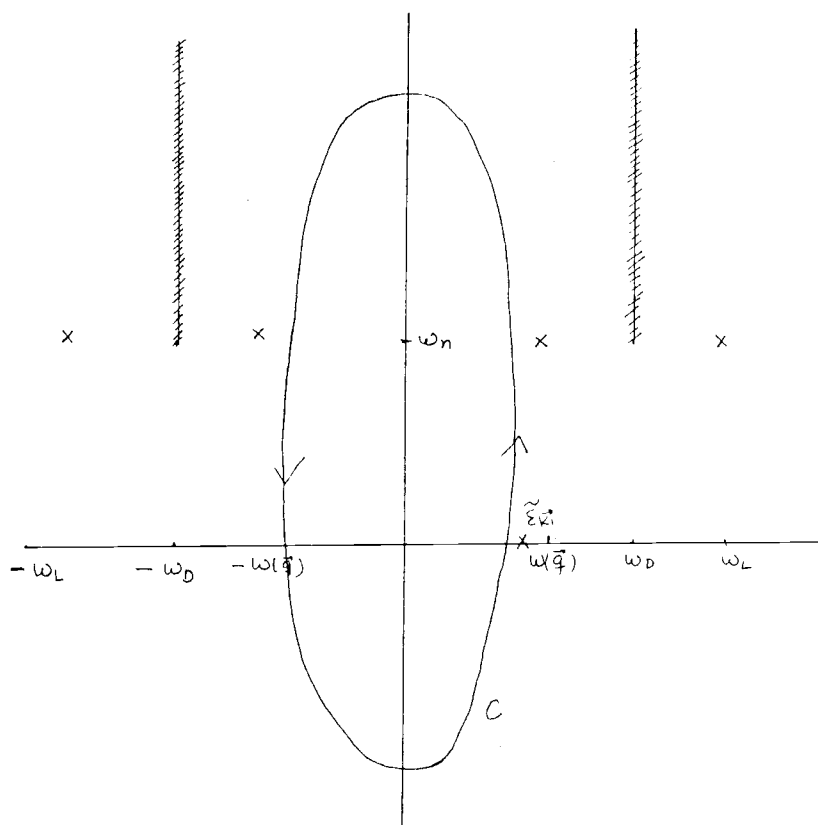


Fig. 4.1

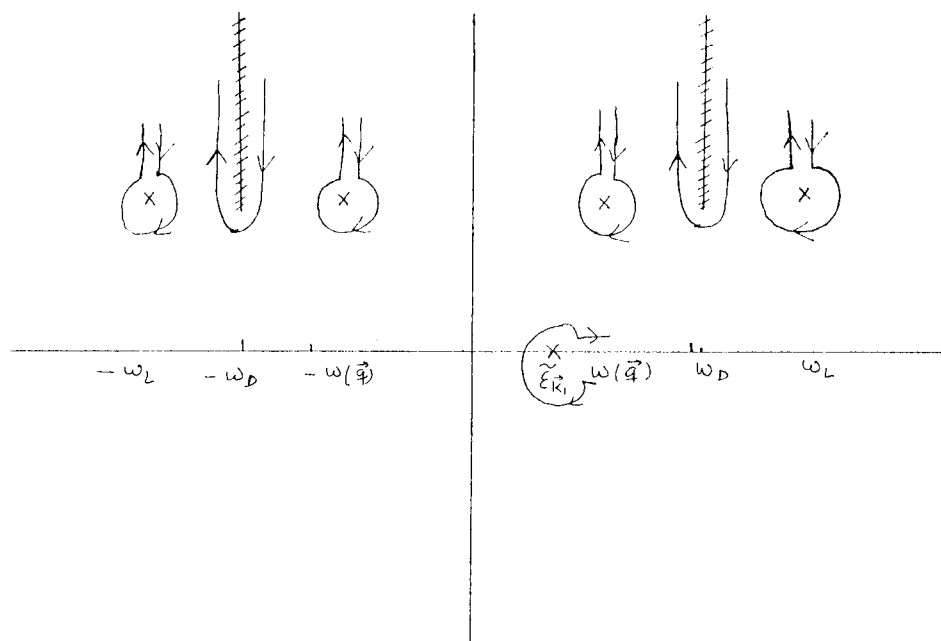


Fig. 4.2

where,

$$f_a(\omega(\vec{q})) = \frac{1 - A \omega^2(\vec{q}) \left[\frac{-\omega(\vec{q})}{2} \ln \left| \frac{-\omega(\vec{q}) + \omega_D}{-\omega(\vec{q}) - \omega_D} \right| - \omega_D \right]}{1 + A \left[\omega^2(\vec{q}) \omega_D + \frac{1}{3} \omega_D^3 + \frac{\omega^3(\vec{q})}{2} \ln \left| \frac{\omega(\vec{q}) - \omega_D}{\omega(\vec{q}) + \omega_D} \right| \right]}$$

and,

$$f_a'(\omega_L) = \frac{1 - A \left[-\frac{\omega_L}{2} \ln \left| \frac{-\omega_L + \omega_D}{-\omega_L - \omega_D} \right| - \omega_D \right]}{A \left[-2(-\omega_L) \omega_D + \frac{(-\omega_L)^3}{\omega_L^2 - \omega_D^2} + \frac{3\omega_L^2}{2} \ln \left| \frac{-\omega_L - \omega_D}{-\omega_L + \omega_D} \right| \right]}$$

Now

$$f(\omega_n + \omega(\vec{q})) = \frac{1}{e^{\beta(\omega_n + \omega(\vec{q}))} + 1} = \frac{1}{-e^{\beta\omega(\vec{q})} + 1} = -\eta(\omega(\vec{q}))$$

and

$$f(\omega_n - \omega(\vec{q})) = \frac{1}{-e^{\beta\omega(\vec{q})} + 1} = 1 + \eta(\omega(\vec{q}))$$

where $\eta(\omega(\vec{q})) = \frac{1}{e^{\beta\omega(\vec{q})} - 1}$ is the Bose function i.e. the average phonon-occupation number.

Similarly, $f(\omega_n + \omega_L) = -\eta(\omega_L)$

$$f(\omega_n - \omega_L) = 1 + \eta(\omega_L)$$

Using these relations, we have

$$\begin{aligned} S_a(\vec{k}_1, \vec{q}) = & \frac{\beta}{m'} \left\{ \left[\frac{f(\tilde{\epsilon}_{\vec{k}_1})}{(\omega_n - \tilde{\epsilon}_{\vec{k}_1})^2 - \omega^2(\vec{q})} \times \right. \right. \\ & \frac{1 - A \omega^2(\vec{q}) \left[\frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1}}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1} + \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_1} - \omega_D} \right| - \omega_D \right]}{1 + A \left[(\omega_n - \tilde{\epsilon}_{\vec{k}_1})^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - \tilde{\epsilon}_{\vec{k}_1})^3}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_1} - \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_1} + \omega_D} \right| \right]} \left. \right] \\ & + \left[\frac{-\eta(\omega(\vec{q}))}{\omega_n + \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}_1}} - \frac{1}{2\omega(\vec{q})} \cdot f_a(\omega(\vec{q})) \right] + \end{aligned}$$

$$\begin{aligned}
& + \left[\frac{1+n(\omega(\vec{q}))}{\omega_n - \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{-2\omega(\vec{q})} \cdot f_a(\omega(\vec{q})) \right] \\
& + \left[\frac{-n(\omega_L)}{\omega_n + \omega_L - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \cdot f_a'(\omega_L) \right] \\
& + \left[\frac{1+n(\omega_L)}{\omega_n - \omega_L - \tilde{\epsilon}_{\vec{k}_i}} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \cdot f_a'(\omega_L) \right]
\end{aligned} \tag{4.6}$$

Substituting the above expression for $S_a(\vec{k}, \vec{q})$ in eq. (3.14) we have

$$\begin{aligned}
\Sigma_a(\vec{k}|\omega_n) = & -\frac{C}{M'} \sum_{\vec{q}, \vec{k}_i} \left\{ \left[\frac{f(\tilde{\epsilon}_{\vec{k}_i})}{(\tilde{\epsilon}_{\vec{k}_i} - \omega_n)^2 - \omega^2(\vec{q})} \times \right. \right. \\
& \left. \frac{1 - A \omega^2(\vec{q}) \left[\frac{\omega_n - \tilde{\epsilon}_{\vec{k}_i}}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_i} + \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_i} - \omega_D} \right| - \omega_D \right]}{1 + A \left[(\omega_n - \tilde{\epsilon}_{\vec{k}_i})^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - \tilde{\epsilon}_{\vec{k}_i})^3}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}_i} - \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}_i} + \omega_D} \right| \right]} \right] \\
& + \left[\frac{n(\omega(\vec{q}))}{\tilde{\epsilon}_{\vec{k}_i} - \omega_n - \omega(\vec{q})} \cdot \frac{1}{2\omega(\vec{q})} \cdot f_a(\omega(\vec{q})) \right] \\
& + \left[\frac{1+n(\omega(\vec{q}))}{\tilde{\epsilon}_{\vec{k}_i} - \omega_n + \omega(\vec{q})} \cdot \frac{1}{2\omega(\vec{q})} \cdot f_a(\omega(\vec{q})) \right] \\
& + \left[\frac{n(\omega_L)}{\tilde{\epsilon}_{\vec{k}_i} - \omega_n - \omega_L} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \cdot f_a'(\omega_L) \right] \\
& + \left[\frac{1+n(\omega_L)}{\tilde{\epsilon}_{\vec{k}_i} - \omega_n + \omega_L} \cdot \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \cdot f_a'(\omega_L) \right] \left. \right\} \times \\
& \Delta^2(\vec{k} - \vec{k}_i) \left[(\vec{k} - \vec{k}_i) \cdot \hat{\epsilon}_S \right]^2
\end{aligned} \tag{4.7}$$

A first principle evaluation of the above equation for $\Sigma_a(\vec{k}|\omega_n)$ (in particular the \vec{k}_1 integration) is analytically not possible. On the other hand, as is commonly done in the theory of superconductivity, it is convenient to take some averages, suitably modified for dHvA studies, over the Fermi surface in order to explore the magnitudes and dependences of the effects being considered. We now change the sum over \vec{k}_1 into an integral, as follows

$$\sum_{\vec{k}_1} = \int_{-\infty}^{\infty} d\tilde{\epsilon}_{\vec{k}_1} \cdot \int \frac{d\vec{k}_1^2}{V_F (2\pi)^3}$$

where V_F is the velocity of the electrons at the Fermi surface. Since $\omega(\vec{q})$ goes only upto ω_D , for large values of $|\tilde{\epsilon}_{\vec{k}_1}|$ the integrand falls off very rapidly. This allows us to extend the lower limit of integration to $-\infty$ without much error. We can now perform the $\tilde{\epsilon}_{\vec{k}_1}$ integration in the complex plane by closing the contour in the upper half-plane to get

$$\begin{aligned} \Sigma_a(\vec{k}|\omega_n) = & -\frac{C}{M'} \sum_{\vec{q}} \int \frac{d\vec{k}_1^2}{V_F (2\pi)^3} (-2\pi i) \left[\left\{ \left[\frac{f(\omega_n + \omega(\vec{q}))}{2\omega(\vec{q})} \mathcal{F}_a(\omega(\vec{q})) \right] \right. \right. \\ & + \left[\frac{f(\omega_n - \omega(\vec{q}))}{-2\omega(\vec{q})} \mathcal{F}_a(\omega(\vec{q})) \right] + \left[\frac{f(\omega_n + \omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) \right] \\ & + \left[\frac{f(\omega_n - \omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \frac{\mathcal{F}_a'(\omega_L)}{(-1)} \right] \\ & \left. \left. + \left[-\frac{1}{\beta} \sum_{m=0}^{\infty} \frac{1}{(2m\pi i k_B T)^2 - \omega^2(\vec{q})} \mathcal{F}_a(2m\pi k_B T i) \right] \right\} \right] \end{aligned}$$

$$\begin{aligned}
& + \left[-\frac{1}{\beta} \sum_{m=1}^n \frac{1}{(2m\pi k_B T i)^2 - \omega^2(\vec{q})} \mathcal{F}_a(2m\pi k_B T i) \right] \Bigg\} \\
& + (-i\pi) \left\{ \frac{1 + 2n(\omega(\vec{q}))}{2\omega(\vec{q})} \mathcal{F}_a(\omega(\vec{q})) + \frac{1 + 2n(\omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) \right\} \Bigg] \times \\
& \left[\Delta^2 + \frac{1 + 2n(\omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) \right] \times \\
& \Delta^2(\vec{k} - \vec{k}_i) \cdot 2k_F^2 (1 - \cos \theta_{\vec{k}\vec{k}_i})
\end{aligned}$$

(4.8)

since $\left[(\vec{k} - \vec{k}_i) \cdot \hat{\varepsilon}_s \right]^2 = 2k_F^2 (1 - \cos \theta_{\vec{k}\vec{k}_i})$ and where it is assumed that $\Delta^2(\vec{k} - \vec{k}_i)$ does not vary much with energy so that it can be considered as constant. We can also take this constant value as the one at the Fermi surface. Now, before doing the surface integration, we note that the residual relaxation time $\tau(\vec{k})$ may be defined by

$$\frac{1}{\tau(\vec{k})} = \sum_{\vec{k}_i} 2\pi N_i \Delta^2(\vec{k} - \vec{k}_i) (1 - \cos \theta_{\vec{k}\vec{k}_i}) \delta(\varepsilon_{\vec{k}_i} - \varepsilon_F) \quad (4.9)$$

where, ε_F is the Fermi energy and N_i is the number of impurity atoms in a unit volume.

Thus writing $c = N_i/N$, we see that we can identify the surface integration as the reciprocal of the relaxation time; remembering that the delta function restriction is already implied in ^{the} derivation. Now considering only the case $n = 0$, as required by our general formulation

we have

$$\begin{aligned}
 \sum_a(\vec{k}|\omega_0) = & -\frac{K_F^2}{M' \pi N} \sum_{\vec{q}} \left[2\pi i \left\{ \frac{1+2n(\omega(\vec{q}))}{2\omega(\vec{q})} \mathcal{F}_a(\omega(\vec{q})) + \right. \right. \\
 & + \frac{1+2n(\omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) + \frac{2\pi i}{\beta} \sum_{m=0}^{\infty} \frac{1}{(2m\pi i k_B T)^2 - \omega^2(\vec{q})} \times \\
 & \left. \mathcal{F}_a(2m\pi k_B T i) \right\} + \\
 & (-i\pi) \left\{ \frac{1+2n(\omega(\vec{q}))}{2\omega(\vec{q})} \mathcal{F}_a(\omega(\vec{q})) + \right. \\
 & \left. \frac{1+2n(\omega_L)}{\omega_L^2 - \omega^2(\vec{q})} \mathcal{F}_a'(\omega_L) \right\} \left. \right] \frac{1}{\tau(\vec{k})}
 \end{aligned} \tag{4.10}$$

$$\begin{aligned}
 \text{Now } & \sum_{m=0}^{\infty} \frac{1}{(2m\pi k_B T i)^2 - \omega^2(\vec{q})} \mathcal{F}_a(2m\pi k_B T i) \\
 = & \frac{1}{2} \left(\frac{\beta}{2\pi i} \right) \int_c \frac{\eta(x)}{x^2 - \omega^2(\vec{q})} \mathcal{F}_a(x) + \frac{1}{2} \frac{1}{-\omega^2(\vec{q})} \mathcal{F}_a(m=0)
 \end{aligned} \tag{4.11}$$

$$\text{where, } \eta(x) = \frac{1}{(e^{\beta x} - 1)}$$

So that after simplification, we find that

$$\sum_a(\vec{k}|\omega_0) = \frac{-K_F^2}{\pi N M'} \sum_{\vec{q}} \frac{i\pi}{\beta \omega^2(\vec{q})} \frac{\left(1 + \frac{3M}{\omega_0^3 \epsilon} \omega^2(\vec{q}) \right)}{(1 + M/\epsilon)} \frac{1}{\tau(\vec{k})}$$

(4.12)

Now carrying out the \vec{q} integration also, using a Debye model,

we finally get

$$\Sigma_a(\vec{k}|\omega_0) = -i \frac{3k_B T}{M'} \frac{k_F^2}{\omega_D^2} \frac{1}{\tau(\vec{k})} \quad (4.13)$$

In the end, we can now define some suitable average, over extremal orbit for example, and write

$$\langle \Sigma_a(\omega_0) \rangle = -i \frac{3k_B T}{M'} \frac{k_F^2}{\omega_D^2} \left\langle \frac{1}{\tau(\vec{k})} \right\rangle_{\text{orbit}} \quad (4.14)$$

where $\langle \dots \rangle_{\text{orbit}}$ here denotes average over some extremal orbit i.e.

$$\left\langle \frac{1}{\tau(\vec{k})} \right\rangle_{\text{orbit}} = \frac{\oint_{\substack{k_z=0 \\ k_{\perp} \text{ on F.S.}}} \frac{dk_{\perp}}{V_{\perp}(\vec{k})} \frac{1}{\tau(\vec{k})}}{\oint_{\substack{k_z=0 \\ k_{\perp} \text{ on F.S.}}} \frac{dk_{\perp}}{V_{\perp}(\vec{k})}} \quad (4.15)$$

where $V_{\perp}(\vec{k})$ is the component velocity of the electron in the orbit plane.

To find the second contribution to the electron self-energy, we have from eq.(3.15)

$$\Sigma_b(\vec{k}|\omega_n) = -\frac{Nc}{s, \vec{q}} \sum_{\omega_n'} \frac{1}{\beta} G_0(\vec{k}-\vec{q}|\omega_n') D_s^d(\vec{q}|\omega_n-\omega_n') \times \\ \left\{ v(\vec{q}) \Delta(-\vec{q}) + v(-\vec{q}) \Delta(\vec{q}) \right\} (\vec{q} \cdot \hat{e}_s)^2 \quad (3.15)$$

Substituting for $D_s^d(\vec{q}|\omega_n-\omega_{n'})$ from eq.(3.12) we get

$$\begin{aligned} \sum_b(\vec{k}|\omega_n) = -N C \sum_{s, \vec{q}} \frac{1}{\beta} \left[\sum_{\omega_{n'}} G_o(\vec{k}-\vec{q}|\omega_{n'}) \frac{M}{M'} \times \right. \\ \left. \left\{ \frac{ds(\vec{q}|\omega_n-\omega_{n'})}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} M \omega_s^2(\vec{q}') ds(\vec{q}'|\omega_n-\omega_{n'})} \right\} \times \right. \\ \left. \left\{ V(\vec{q}) \Delta(-\vec{q}) + V(-\vec{q}) \Delta(\vec{q}) \right\} (\vec{q} \cdot \hat{\epsilon}_s)^2 \right] \quad (4.16) \end{aligned}$$

For convenience denoting the $\omega_{n'}$ sum in the square bracket by $S_b(\vec{k}-\vec{q})$ and using an isotropic phonon spectrum, we have

$$\begin{aligned} S_b(\vec{k}-\vec{q}) = \sum_{\omega_{n'}} \frac{1}{\omega_{n'} - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{M}{M'} \frac{1}{M} \cdot \frac{1}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q})} \times \\ \left\{ \frac{1}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{\omega^2(\vec{q}')}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q}')}} \right\} \quad (4.17) \end{aligned}$$

where as before $\tilde{\epsilon}_{\vec{k}-\vec{q}} = (\epsilon_{\vec{k}-\vec{q}} - \mu)$

Converting the sum over $\omega_{n'}$ in to a contour integral, as in the case of $\sum_a(\vec{k}|\omega_n)$ and then, deforming the contour in the same way we pick up contributions from the poles of electron Green's function and phonon Green's function including the 'localized mode', if any. The result of all this is

$$\begin{aligned} S_b(\vec{k}-\vec{q}) = \frac{1}{M'} \left\{ \left[\frac{f(\tilde{\epsilon}_{\vec{k}-\vec{q}})}{(\omega_n - \tilde{\epsilon}_{\vec{k}-\vec{q}})^2 - \omega^2(\vec{q})} \right] \times \right. \\ \left. \left\{ \frac{1}{1 + A [(\omega_n - \epsilon_{\vec{k}-\vec{q}})^2 \omega_D + \frac{1}{3} \omega_D^3 + \frac{(\omega_n - \epsilon_{\vec{k}-\vec{q}})^3}{2} \ln \left| \frac{\omega_n - \tilde{\epsilon}_{\vec{k}-\vec{q}} - \omega_D}{\omega_n - \tilde{\epsilon}_{\vec{k}-\vec{q}} + \omega_D} \right|]} \right\} \right. \\ \left. + \left[\frac{-\eta(\omega(\vec{q}))}{\omega_n + \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{1}{2\omega(\vec{q})} \cdot f_b(\omega(\vec{q})) \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + \left[\frac{1 + n(\omega(\vec{q}))}{\omega_n - \omega(\vec{q}) - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{1}{2\omega(\vec{q})} \mathcal{F}_b(\omega(\vec{q})) \right] \\
& + \left[\frac{-n(\omega_L)}{\omega_n + \omega_L - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{1}{-2\omega(\vec{q})} \mathcal{F}_b(\omega(\vec{q})) \right] \\
& + \left[\frac{-n(\omega_L)}{\omega_n + \omega_L - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \frac{\mathcal{F}_b'(\omega_L)}{(-1)} \right] \\
& + \left[\frac{1 + n(\omega_L)}{\omega_n - \omega_L - \tilde{\epsilon}_{\vec{k}-\vec{q}}} \frac{1}{\omega_L^2 - \omega^2(\vec{q})} \frac{\mathcal{F}_b'(\omega_L)}{(1)} \right] \Bigg\} \quad (4.18)
\end{aligned}$$

where,

$$\mathcal{F}_b(\omega(\vec{q})) = 1 / \left\{ 1 + A \left[\omega^2(\vec{q}) \omega_D + \frac{1}{3} \omega_D^3 + \frac{\omega^3(\vec{q})}{2} \ln \left| \frac{\omega(\vec{q}) - \omega_D}{\omega(\vec{q}) + \omega_D} \right| \right] \right\}$$

and,

$$\mathcal{F}_b'(\omega_L) = 1 / \left[2\omega_L \omega_D + \frac{\omega_L^3 \omega_D}{\omega_L^2 - \omega_D^2} + \frac{3\omega_L^2}{2} \ln \left| \frac{\omega_L - \omega_D}{\omega_L + \omega_D} \right| \right]$$

In terms of $S_b(\vec{k} - \vec{q})$ we can write $\Sigma_b(\vec{k} | \omega_n)$ as

$$\begin{aligned}
\Sigma_b(\vec{k} | \omega_n) &= -Nc \sum_{\vec{q}} S_b(\tilde{\epsilon}_{\vec{k}-\vec{q}}, \omega(\vec{q})) \times \left\{ V(\vec{q}) \Delta(-\vec{q}) + V(-\vec{q}) \Delta(\vec{q}) \right\} \times \\
&\quad \left\{ \sum_s (\vec{q} \cdot \hat{e}_s)^2 \right\} \quad (4.19)
\end{aligned}$$

If we restrict ourselves to normal processes¹, then a sum over \vec{q} is

1. The ensemble averaging actually gives delta function restrictions for both 'normal' and 'umklapp' processes. Umklapp processes are no doubt important for resistivity, where large angle scattering dominates; however, for dHvA effect their effect may not be as big as in resistivity. In any case, because of the parametrization that we do, the effect of umklapp processes can also be taken into account in the end.

equivalent to a sum over \vec{k}_1 , since in this case $\vec{q} = (\vec{k} - \vec{k}_1)$. This allows us to write (for a unit volume)

$$\sum_{\vec{k}_1} = \int_{-\infty}^{\infty} d\tilde{\epsilon}_{\vec{k}_1} \int \frac{dk_1^2}{V_F (2\pi)^3} \quad (4.20)$$

where V_F is the velocity of the electrons at the Fermi surface. It is also convenient to separate the phonon contribution by introducing a delta function. We have

$$\begin{aligned} \Sigma_b(\vec{k}|\omega_n) = -Nc \int_{-\infty}^{\infty} d\tilde{\epsilon}_{\vec{k}_1} \int \frac{dk_1^2}{V_F (2\pi)^3} \int_0^{\infty} d\omega \delta(\omega - \omega_{\vec{k}-\vec{k}_1}) \times \\ S_b(\tilde{\epsilon}_{\vec{k}_1}, \omega_{\vec{k}-\vec{k}_1}) \left\{ V(\vec{k}-\vec{k}_1) \Delta(\vec{k}_1-\vec{k}) + V(\vec{k}_1-\vec{k}) \Delta(\vec{k}-\vec{k}_1) \right\} \\ \times \left\{ (\vec{k}-\vec{k}_1) \cdot \hat{\epsilon}_s \right\}^2 \end{aligned} \quad (4.21)$$

Now performing the $\tilde{\epsilon}_{\vec{k}_1}$ integration by closing the contour in the upper half plane, we find

$$\begin{aligned} \Sigma_b(\vec{k}|\omega_n) = -\frac{Nc}{M'} \int \frac{dk_1^2}{V_F (2\pi)^3} \int_0^{\infty} d\omega \delta(\omega - \omega_{\vec{k}-\vec{k}_1}) (-2\pi i) \\ \left\{ \left[\frac{f(\omega_n + \omega_L)}{\omega_L^2 - \omega^2} \mathcal{F}_b'(\omega_L) + \frac{f(\omega_n - \omega_L)}{\omega_L^2 - \omega^2} \mathcal{F}_b'(\omega_L) \right] \right. \\ + \left[\frac{f(\omega_n + \omega)}{2\omega} \mathcal{F}_b(\omega) + \frac{f(\omega_n - \omega)}{-2\omega} \mathcal{F}_b(\omega) \right] \\ + \left[-\frac{1}{\beta} \sum_{m=0}^{\infty} \frac{1}{(2m\pi k_B T i)^2 - \omega^2} \mathcal{F}_b(2m\pi k_B T i) \right] \\ \left. + \left[-\frac{1}{\beta} \sum_{m=1}^n \frac{1}{(2m\pi k_B T i)^2 - \omega^2} \mathcal{F}_b(2m\pi k_B T i) \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + i \pi \left[\frac{-n(\omega)}{2\omega} f_b(\omega) - \frac{1+n(\omega)}{2\omega} f_b(\omega) - \right. \\
& \quad \left. \frac{1+2n(\omega_L)}{\omega_L^2 - \omega^2} f_b'(\omega_L) \right] \Big\} \times \\
& 2 \operatorname{Re} \left[V(\vec{k}-\vec{k}_i) \Delta(\vec{k}_i-\vec{k}) \right] \left[\sum_s (\vec{k}-\vec{k}_i) \cdot \hat{\epsilon}_s \right]^2
\end{aligned} \tag{4.22}$$

Considering only the $n = 0$ case, as is required by our general formulation, we get after simplifying

$$\begin{aligned}
\Sigma_b(\vec{k}|\omega_0) &= -\frac{Nc}{M'} \int d\omega \delta(\omega - \omega_{\vec{k}-\vec{k}_i}) \int \frac{dk_i^2}{V_F (2\pi)^3} \frac{i\pi}{\beta \omega^2} \frac{1}{(1+M/E)} \times \\
& 2 \operatorname{Re} \left[V(\vec{k}-\vec{k}_i) \Delta(\vec{k}_i-\vec{k}) \right] \left[\left(\sum_s (\vec{k}-\vec{k}_i) \cdot \hat{\epsilon}_s \right) \right]^2
\end{aligned} \tag{4.23}$$

Now using the relation for the electron-phonon coupling constant in terms of the scattering potential⁽²⁰⁾

$$\left| \bar{g}_s(\vec{k}-\vec{k}_i) \right|^2 = \frac{N}{2M\omega_{\vec{k}-\vec{k}_i}} \left| V(\vec{k}-\vec{k}_i) \cdot \sum_s (\vec{k}-\vec{k}_i) \cdot \hat{\epsilon}_s \right|^2 \tag{4.24}$$

we can write $\Sigma_b(\vec{k}|\omega_n)$ as

$$\begin{aligned}
\Sigma_b(\vec{k}|\omega_0) &= -\frac{2Nc}{M'} \int \frac{dk_i^2}{V_F (2\pi)^3} \int d\omega \delta(\omega - \omega_{\vec{k}-\vec{k}_i}) \times \\
& \frac{i\pi}{\beta \omega^2} \frac{1}{(M/M')} \cdot \frac{2M}{N} \omega_{\vec{k}-\vec{k}_i} \left[\bar{g}(\vec{k}-\vec{k}_i) \Delta \bar{g}(\vec{k}_i-\vec{k}) \right]
\end{aligned} \tag{4.25}$$

Finally, taking the average over \vec{k} , at the extremal orbit $k_z=0$, we arrive at

$$\left\langle \Sigma_b(\omega) \right\rangle_{\text{orbit}} = -\frac{C}{\beta} (2\pi i) \int_0^{\infty} d\omega \left\langle \frac{2 [\bar{g}(\omega) \Delta \bar{g}(\omega)] F(\omega)}{\omega} \right\rangle_{\text{orbit}} \quad (4.26)$$

where $F(\omega)$ is the phonon density of states and analogous to the theory of super-conductivity, we have defined

$$\begin{aligned} \left\langle \bar{g}(\omega) \Delta \bar{g}(\omega) F(\omega) \right\rangle_{\text{orbit}} &= \oint_{\substack{k_z=0 \\ k_{\perp} \text{ on F.S.} \\ \text{extremal orbit}}} \frac{dk_{\perp}}{V_{\perp}(\vec{k})} \cdot \frac{\int \frac{dk_{\perp}^2}{V_F(2\pi)^3} \left[\bar{g}(\vec{k}-\vec{k}_1) \Delta \bar{g}(\vec{k}-\vec{k}_1) \right] \times}{\delta(\omega - \omega_{\vec{k}-\vec{k}_1})} \\ &= \oint_{\substack{k_z=0 \\ k_{\perp} \text{ on F.S.} \\ \text{extremal orbit}}} \frac{dk_{\perp}}{V_{\perp}(\vec{k})} \end{aligned} \quad (4.27)$$

Thus the new parameter that appears in the interference term has the product $\bar{g}(\omega) \Delta \bar{g}(\omega)$ instead of $\bar{g}^2(\omega)$ which appear in the unperturbed system.

The third contribution to the electron self-energy $\Sigma_c(\vec{k}|\omega_n)$ from eq. (3.16) is

$$\begin{aligned} \Sigma_c(\vec{k}|\omega_n) &= -N \sum_{\vec{s}, \vec{k}_1, \vec{q}} \frac{1}{\beta} \sum_{\omega_n'} G_0(\vec{k}_1|\omega_n') D_S(\vec{q}|\omega_n - \omega_n') \times \\ &\quad \frac{\vec{q} = \vec{k} - \vec{k}_1 + \vec{q}}{V^2(\vec{k} - \vec{k}_1) \left[(\vec{k} - \vec{k}_1) \cdot \hat{\epsilon}_s \right]^2} \end{aligned} \quad (4.28)$$

Considering only the normal processes, as before, and denoting

$S_c(\vec{k}_1 | \vec{q}) = \sum_{\omega_{n'}} G_o(\vec{k}_1 | \omega_{n'}) D_s(\vec{q} | \omega_n - \omega_{n'})$ we have, for an isotropic phonon spectrum

$$\begin{aligned}
 S_c(\vec{k}_1 | \vec{q}) &= \sum_{\omega_{n'}} G_o(\vec{k}_1 | \omega_{n'}) D(\vec{q} | \omega_n - \omega_{n'}) \\
 &= \sum_{\omega_{n'}} G_o(\vec{k}_1 | \omega_{n'}) d(q | \omega_n - \omega_{n'}) \times \\
 &\quad \left\{ \frac{1 + \frac{M}{\epsilon} c - (1-c) \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{M \omega^2(\vec{q}')}{\omega_n - \omega_{n'}} d(\vec{q} | \omega_n - \omega_{n'})}{1 - \frac{M}{\epsilon} c \frac{\omega^2(\vec{q})}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q})} - (1-c) \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{\omega^2(\vec{q}')}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q}')}} \right\} \quad (4.29)
 \end{aligned}$$

Because for dHVA effect the impurity concentration is typically of the order of 1 %, we would be interested only in terms which are linear in concentration. Rearranging the denominator and expanding it, assuming c small, we get (upto terms linear in concentration)

$$\begin{aligned}
 S_c(\vec{k}_1 | \vec{q}) &= \sum_{\omega_{n'}} G_o(\vec{k}_1 | \omega_{n'}) d(\vec{q} | \omega_n - \omega_{n'}) \times \\
 &\quad \left\{ 1 + \frac{\frac{M}{\epsilon} c}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{\omega^2(\vec{q}')}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q}')}} + \right. \\
 &\quad \left. \frac{1}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q})} \times \frac{\frac{M}{\epsilon} c \omega^2(\vec{q})}{1 - \frac{M}{\epsilon} \frac{1}{N} \sum_{\vec{q}'} \frac{\omega^2(\vec{q}')}{(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q}')}} \right\} \quad (4.30)
 \end{aligned}$$

The third term in the above sum has a double pole and it is convenient to evaluate it by the following approximate procedure rather than by contour integration. Because the function $\frac{\omega^2(\vec{q}')}{[(\omega_n - \omega_{n'})^2 - \omega^2(\vec{q}')]^2}$ is very sharply peaked near $(\omega_n - \omega_{n'}) = 0$, most of the contribution to the integral will come from the region close to this. Hence, using $(\omega_n - \omega_{n'}) = 0$ in the last term of the above eq. (4.30), we find that its contribution is

$$= \sum_{\omega_n'} G_{10}(\vec{R}_1 | \omega_n) \frac{M}{\epsilon} \frac{1}{\omega^2(\vec{q})} \frac{1}{(1 + \frac{M}{\epsilon})} \quad (4.31)$$

which, as we can easily verify, will give a contribution to the self-energy that exactly cancels the contribution from the second term. Thus to lowest order in concentration, the contribution from $\Sigma_c(\omega_0)$ is only from the host atoms without any modification i.e.

$$\begin{aligned} \Sigma_c(\omega_0) &= -i \pi k_B T \int \frac{2 \vec{q}^2(\omega) F(\omega)}{\omega} d\omega \\ &= -i \pi k_B T \lambda_h \end{aligned} \quad (4.32)$$

It is interesting to note that the approximation that we used above in evaluating the last term in eq.(4.30) may indeed be a very good one, because if we use the same approximation in the second term of the same eq.(4.30) we get exactly the same result as we get by doing the contour integration. Thus there is some cancellation effect which all the more seems to justify our approximation.

V. RESULTS AND DISCUSSION

In chapter II we presented a new derivation of the basic formula for the dHvA effect, in particular for the dHvA amplitude. We have been successful in extending the calculations of Fowler and Prange⁽⁵⁾, which is essentially a high temperature calculation to lower temperatures by approximately summing contributions from all the poles of the Fermi function on the imaginary energy axis. Now in our new formula, there explicitly appears the divergent effects at very low temperatures that one finds in the work of Engelsberg and Simpson who tried to sum over all the poles on the imaginary axis numerically. Moreover the form that we obtained is a simple algebraic closed form, which seems to be highly useful in understanding the basic character of the dHvA oscillations.

We see from the analysis of chapter II that the dHvA effect is an extremely unusual and useful experiment. First, as we pointed out earlier the amplitude and frequency of the oscillations depend on the imaginary and real part of the self-energy respectively for any short range interaction potential. For electron-phonon interaction we know that the real part of the self-energy on the imaginary energy axis is zero. This then has the consequence that the band-mass of the electron which occurs in the frequency of dHvA oscillations is not affected by the electron-phonon (el-ph) interactions. Thus, by measuring the band-mass by frequency measurements and el-ph enhanced band-mass by amplitude measurements, one can measure the el-ph enhancement factor λ . Since the enhancement factor, thus obtained, does not depend on temperature one can measure it

in any temperature range in which dHvA experiments can be done. This then provides very much of flexibility from the experimental point of view.

From the explicit calculations of chapter IV, we find that the el-ph self-energy, even in a dilute disordered alloy, has its imaginary part linearly proportional to temperature. On the other hand the self-energy due to scattering from the fixed impurities is, to a good approximation independent of temperature. Thus the temperature independent self-energy shows up in the form of 'Dingle temperature' and causes a reduction in the amplitude of oscillations. For the el-ph self-energy the linear temperature dependence has the effect that it simply enhances the electron mass. Thus, the two self-energies (one temperature dependent and other independent) can be investigated separately. In this regard we like to point out that whereas some authors⁽²⁴⁾ believe that the el-ph enhanced mass should be used in the co-efficient of Dingle temperature others⁽¹³⁾ think that only the band-mass should be used there. As an application of our earlier derivation of Dingle temperature, we show below that at least in the zero temperature limit, the mass used in the co-efficient of Dingle temperature is not the el-ph enhanced mass.

Consider eq.(2.44) again, but now let us modify the electron lines to include renormalization due to phonon scattering. We get for the el-ph self-energy due to static impurity

$$\Sigma^{\text{imp}}(i\omega_n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\Gamma(\omega) d\omega}{i\omega_n - (\omega - i\lambda) - \Sigma_{\text{el-ph}}(i\omega_n)}$$

(5.1)

and, therefore, the imaginary part, evaluated at the first pole on the imaginary energy axis, is

$$\text{Im } \Sigma^{\text{imp}}(i\omega_0) = -\frac{\omega_0(1+\lambda)}{2\pi} \int_{-\infty}^{\infty} \frac{\Gamma(\omega) d\omega}{(1+\lambda)^2 \omega_0^2 + (\omega - i\lambda)^2} \quad (5.2)$$

since $\Sigma_{\text{el-ph}}(i\omega_0) = -i\omega_0\lambda$.

Now if we take the limit $T \rightarrow 0$, we find that the el-ph renormalization effects go away, and we get back the original unmodified expression for the Dingle temperature. This is one of the very important results of the new approach. It may be remarked here that the above process can be done self-consistently by including the static impurity self-energy also in the renormalization process, but that should not change the conclusions already drawn.

We feel that the new derivation will have useful application in the theory of steady diamagnetism. Where, for example, one can possibly extend our arguments and derive the theorem that el-ph interactions do not contribute to steady diamagnetism. This theorem arises from the fact that the el-ph self-energy has no real part when evaluated on the imaginary energy axis. We also feel that the concepts developed in the new derivation will be useful in more detailed studies of magnetic breakdown in metals.

In chapter IV we derived explicitly the various expressions for el-ph self-energy in a dilute substitutional binary alloy. We included

both effects arising from changes in the el-ph coupling and mass associated with the impurity. To order linear in concentration, there are two terms, which appear as corrections to the el-ph enhanced effective mass in the host. One due to scattering from impurity site displacement, and other due to successive scattering from host and impurity atoms respectively or vice-versa. Whereas the first correction (due to $\Sigma_a(\omega_n)$) is always positive, the correction due to the second term can be positive or negative depending on the valence difference of the impurity from the host. It is also clear that in general these corrections depend on the orbital averages considered. The effective mass parameter λ now, in the impure system, is given by

$$\lambda = \frac{-\partial \Sigma(i\omega_n)}{\partial(i\omega_n)} = \frac{-\partial [\Sigma_a(i\omega_n) + \Sigma_b(i\omega_n) + \Sigma_c(i\omega_n)]}{\partial(i\omega_n)} \quad (5.3)$$

for $n = 0$ case, we get

$$\lambda = \left[\frac{3k_F^2}{M' \omega_D^2} \left\langle \frac{1}{\tau(\vec{k})} \right\rangle_{orbit} + 2C \cdot \int_0^\infty \left\langle \frac{\bar{g}(\omega) \Delta \bar{g}(\omega) F(\omega)}{\omega} \right\rangle_{orbit} d\omega + \lambda_h \right] \quad (5.4)$$

where λ_h is the enhancement factor in the host. If we denote the first two correction terms on the right hand side of eq (5.4) by λ_a and λ_b respectively, we have

$$\lambda_a = \frac{3 k_F^2 \hbar}{M' \omega_D^2} \left\langle \frac{1}{z(\vec{k})} \right\rangle_{\text{orbit}} \quad (5.5)$$

where we have restored \hbar back(which was taken as unity throught in the text) and

$$\lambda_b = 2c \int_0^\infty \left\langle \frac{\bar{g}(\omega) \Delta \bar{g}(\omega) F(\omega)}{\omega} \right\rangle d\omega \quad (5.6)$$

In general the coefficient of the residual relaxation time in eq.(5.5) is small.Using the datas given in "Introduction to Solid State Physics"(fourth edition) by Kittel,we find that the factor has the following values

$$\begin{aligned} \text{for, Au-Ag} & \quad 5 * 10^{-17} \text{ sec.}, \\ \text{and for, Mg-Al} & \quad 2 * 10^{-16} \text{ sec.} \end{aligned}$$

The average reciprocal-relaxation time in these alloys is of the order of 10^{13} sec^{-1} .It appears ,therefore, that the effect is too small to be measurable.However,we note that the measured transport relaxation time is usually an average over the entire Fermi surface,whereas the residual relaxation time which occurs in eq (5.4) is an average over some orbit.Because of anisotropy,it is quite possible that this factor (ie. $\left\langle \frac{1}{z(\vec{k})} \right\rangle_{\text{orbit}}$) may be large ^{for} some orbits.In such cases one may observe an appreciable enhancement of the el-ph mass.This seems to be the case in the experiments of Tripp and co-workers⁽²²⁾.In alloy of 0.8 % Cu in Be

Tripp et al found that⁽²⁴⁾ there was about 50 % enhancement of the electron's effective mass for the neck orbit. We can suggest one other system in which the effect may be measurable. Because Sn has a reasonably high Fermi energy and reasonably low Debye temperature, it may be a good substance in which the addition of a light impurity like Mg or Be should give a measurable change in the enhancement factor on alloying.

The second term λ_b is directly proportional to the concentration and, for dHvA experiments, is small in general. However, if the change in the electron-phonon coupling constant, $\Delta\bar{g}(\omega)$, is large, then this term may also give rise to a measurable effect.

BIBLIOGRAPHY

1. Abrikosov, A.A., Gorkov, L.P. and Dzyaloshinski, I.E. 'Methods of Quantum Field Theory in Statistical Physics'. Translated and edited by R.A. Silverman (Prentice Hall Inc., Englewood cliffs, New Jersey, 1963) ch.3.
2. Ambegaonkar, V., 'Green's Functions in Many-Body Problems' in Astrophysics and the Many-Body Problem. vol. 2 of the 1962 Brandeis Summer Institute. Published by W.A. Benjamin Inc., New York. p321.
3. Dingle, R.B., 'Some magnetic properties of metals II- The influence of collisions on the magnetic behaviour of large systems.' Proc. Roy. Soc. A 211, (1952), 517.
4. Englesberg, S. and Simpson, G., 'Influence of Electron-Phonon Interactions on the de Haas-van Alphen Effect.' Phys.Rev. B2, (1970) 1657.
5. Fowler, M. and Prange, R.E., 'Electron-Phonon renormalization effects in high magnetic fields; The de Haas-van Alphen Effect.' Physics vol.1, no.6 (1965), 315.
6. Fetter, A.L. and Walecka, J.D., 'Quantum Theory of Many Particle Systems.' McGraw Hill Book Co. (1971).
7. Hicks, J.C., 'Electron-Phonon contribution to the electronic density of states in a dilute alloy.' Ph.D. Thesis, Oregon State University (1974).
8. Kagan, Yu and Zhernov, A.P., 'Contribution to the theory of electric conductivity of metals with non-magnetic impurities.' Soviet Physics, JETP. vol.23, no 4 (1966), 737.
9. Luttinger, J.M., 'Theory of the de Haas-van Alphen effect for a system of interacting fermions.' Phys.Rev. 121 (1961), 1251.
10. Luttinger, J.M. and Ward, J.C., 'Ground state energy of a many fermion system II.' Phys.Rev. 118 (1960), 1417.
11. Lifshitz, I.M. and Kosevich, A.M., 'Theory of Magnetic Susceptibility in metals at Low Temperatures.' Sov.Phys. JETP. 2(1956), 636.
12. Lee, T.D. and Yang, C.N., 'Many body Problems in Quantum Statistical Mechanics IV. Formulation in Terms of Average Occupation Number in Momentum Space.' Phys.Rev. 117 (1960), 22.
13. Lowndes, D.H., et al, 'Maps of Electronic Life time Anisotropy for Dilute Alloys of Ag, Cu, Zn and Fe in Au from dHvA Dingle Temperature measurements.' Low Temperature Physics-LTL3. vol 4, (1974) Plenum Press, New York; p201.

14. McMillan, W.L., 'Transition temperature of strong coupled superconductors.' Phys. Rev., 167 (1968), 331.
15. Migdal, A.B., 'Interaction between Electrons and Lattice Vibrations in a Normal Metal.' Sov. Phys. JETP, vol. 34(7) no 6, (1956), 996.
16. Palin, C.J., et al, 'Amplitudes in the de Haas-van Alphen effect.' Proceedings of the twelfth international conference on low temperature physics. LT 12, (1971), 513.
17. Rice, T.M., 'The effects of Electron-Electron Interactions on the Properties of Metals.' Annals of Phys. (New York) 31, (1965), 100.
18. Sham, L.J. and Ziman, J.M., 'The electron-phonon interaction.' in Solid State Physics; edited by F. Seitz and D. Turnbull (Academic Press, Inc. New York, 1963), vol. 15, 221.
19. Soven, Paul, 'Theory of the de Haas-van Alphen effect in dilute alloys.' Phys. Rev. B5, (1972), 260.
20. Scalapino, D.J., 'The electron-phonon interaction and strong coupling superconductors.' in Superconductivity, vol. 1; edited by R.D. Parks (1969), 449.
21. Taylor, P.L., 'Electronic specific heat of dilute alloys.' Phys. Rev. 178, (1969), 918.
22. Tripp, J.H., et al, 'Effect of alloying on the Fermi surface of Beryllium.' Phys. Rev. B2, (1970), 1556.
23. Harris, R., 'Calculations of de Haas-van Alphen Life times in Copper-Based Alloys.' Low Temperature Physics-LT 13, vol. 4, (1974). Plenum Press, New York, p 241.
24. Coleridge, P.T., 'De Haas-van Alphen Effect and Fermi surface changes in dilute alloys.' Low Temperature Physics, LT 13, vol. 4, (1974). Plenum Press, New York, p9.
25. Wasserman, A., 'Evaluation of Some Fermi-Dirac Integrals.' J. of Mathematical Physics, vol. 11, (1970), 477.
26. Shoenberg, D., 'Evidence from the de Haas-van Alphen Effect.' Phys. Kondens Materie 9, (1969), 1.

APPENDICES

A. DE HAAS-VAN ALPHEN EFFECT

Consider a large pure crystal in a magnetic field directed along the z-axis. In the one electron approximation, the Schrödinger equation of an electron (disregarding spin for the moment) can be written as

$$\frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 \psi + V(\vec{r}) \psi = E \psi \quad (\text{A-1})$$

where $\vec{B} = \text{Curl } \vec{A}$, and we choose the gauge such that $\vec{A} = (0, xB, 0)$. $V(\vec{r})$ is the potential energy of the electron in the periodic lattice-potential. In a very rough approximation (which is good in many cases at least for electrons near the Fermi surface) the influence of the lattice can be taken into account by replacing the free electron mass by an effective mass called the band-mass. Since the main behaviour of the electron is not affected by this approximation, we will use \hbar in the following. Thus assuming that m now represents the band-mass, eq. (A-1) reduces to

$$\frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 \psi = E \psi \quad (\text{A-2})$$

Expanding the bracket and remembering that, in the gauge chosen, \vec{p} commutes with \vec{A} , we get

$$\left(\frac{p^2}{2m} - \frac{e}{mc} (\vec{A} \cdot \vec{p}) + \frac{e^2}{2mc^2} A^2 \right) \psi = E \psi \quad (\text{A-3})$$

Replacing \vec{p} by its explicit operator form $\vec{p} = -i \hbar \nabla$ and using $\vec{A} = (0, xB, 0)$ we get

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) \psi + \left(\frac{\partial}{\partial y} - \frac{ieBx}{\hbar c} \right)^2 \psi + \frac{2mE}{\hbar^2} \psi = 0$$

$$\psi(x, y, z) = e^{i(k_y y + k_z z)} U(x) \quad (\text{A-4})$$

The solution of this will be of the form

$$\psi(x, y, z) = e^{i(k_y y + k_z z)} U(x) \quad (\text{A-5})$$

Using (A-5) in (A-4) we get the condition on $U(x)$

$$\frac{\partial^2 U(x)}{\partial x^2} + \left\{ \frac{2mE'}{\hbar^2} - \left(k_y - \frac{eB}{\hbar c} x \right)^2 \right\} U(x) = 0 \quad (\text{A-6})$$

with

$$E' = \left(E - \frac{\hbar^2}{2m} k_z^2 \right) \quad (\text{A-7})$$

From (A-4) it is clear that the motion of the electron in the z -direction is exactly like a free electron; however, for motion in the x - y plane we have to solve the differential eq. (A-6). Rewriting it as

$$-\frac{\hbar^2}{2m} \frac{\partial^2 U(x)}{\partial x^2} + \frac{1}{2} m \left(\frac{eB}{m c} x - \frac{\hbar k_y}{m} \right)^2 U(x) = E' U(x) \quad (\text{A-8})$$

we note that this is the equation of a one dimensional harmonic oscillator with frequency

$$\omega_c = \frac{eB}{m c}$$

centered on the point

$$x_0 = \left(\frac{1}{\omega_c} \frac{\hbar k_y}{m} \right)$$

Thus

$$\varepsilon' = \left(n + \frac{1}{2}\right) \hbar \omega_c$$

and

$$\varepsilon = \left(n + \frac{1}{2}\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m} = \varepsilon_{n,k_z}$$

when spin is also included, we get

$$\varepsilon_{n,k_z,\sigma} = \left(n + \frac{1}{2}\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m} + \sigma g \mu_B B \quad (\text{A-9})$$

where $\sigma = \pm \frac{1}{2}$ and $\mu_B = \frac{e \hbar}{2 m c}$

These $\varepsilon_{n,k_z,\sigma}$ are the Landau levels of an electron in a magnetic field. Since $\omega_c = (eB/mc)$, the energy of these levels directly depends on the magnetic field and they become wider and move up as the strength of the magnetic field increases.

Another important thing about these levels is their degeneracy, which is given by

$$p = \frac{m \omega_c}{2 \pi \hbar^2} L_x L_y = \frac{e B}{2 \pi \hbar^2 c} L_x L_y \quad (\text{A-10})$$

where L_x, L_y, L_z are the dimensions of the crystal. The degeneracy of each level is thus also a function of the magnetic field. As the magnetic field increases the energy level starts to move up and the energy of the system increases, but the degeneracy of each level is also increasing at the same time. When the topmost level starts crossing the Fermi surface it begins to empty, because the lower levels now can hold more electrons; and while it is emptying the energy of the system decreases. Thus the free energy of the system oscillates which in

turn gives rise to oscillations in the magnetic susceptibility:The
de Haas-van Alphen Effect.

B. LINE INTEGRAL

In chapter IV while evaluating $\sum_a(\vec{k}|\omega_n)$ by contour integration technique, we said that the integrals around the branch cuts are negligible. In this appendix we show this explicitly. We have for the line integral which arises in the evaluation of $\sum_a(\vec{k}|\omega_n)$ as

$$I = \int_L dx \frac{f(x)}{x - \tilde{\epsilon}_{\vec{k}_1}} \frac{1}{(x - \omega_n)^2 - \omega^2(\vec{q})} \frac{1 + A \omega^2(\vec{q}) \left[\frac{x - \omega_n}{2} \ln \left| \frac{x - \omega_n - \omega_D}{x - \omega_n + \omega_D} \right| - \omega_D \right]}{1 + A \left[(x - \omega_n)^2 \omega_D + \frac{1}{3} \omega_D^3 - \frac{(x - \omega_n)^3}{2} x \ln \left| \frac{x - \omega_n + \omega_D}{x - \omega_n - \omega_D} \right| \right]} \quad (B-1)$$

The branch points are at $x = \omega_n \pm \omega_D$ and we take the branch cuts as shown in fig. (4.1). Let us first evaluate the line integral around the branch point at $x = \omega_n + \omega_D$. To do this let us put

$$\begin{aligned} x - \omega_n - \omega_D &= iy \\ dx &= i dy \end{aligned}$$

we get, denoting this part of the integral by I_1 ,

$$I_1 = \int_{L_1} dx \frac{f(iy + \omega_n + \omega_D)}{(iy + \omega_n + \omega_D - \tilde{\epsilon}_{\vec{k}_1})} \frac{1}{(iy + \omega_D)^2 - \omega^2(\vec{q})} \frac{x}{1 + A \omega^2(\vec{q}) \left[\frac{iy + \omega_D}{2} \ln \left| \frac{iy}{iy + 2\omega_D} \right| - \omega_D \right]} \quad (B-2)$$

$$1 + A \left[(iy + \omega_D)^2 \omega_D + \frac{1}{3} \omega_D^3 - \frac{(iy + \omega_D)^3}{2} \ln \left| \frac{iy + 2\omega_D}{iy} \right| \right]$$

For large y the integrand goes as $(1/y^5)$, therefore any

C. LIST OF FREQUENTLY USED SYMBOLS

| SYMBOL | MEANING |
|------------|---|
| e | charge of an electron |
| m | effective band-mass of an electron |
| h | Planck's constant |
| \hbar | Planck's constant h divided by 2π |
| k_B | Boltzmann constant |
| T | Absolute temperature |
| β | $1/k_B T$ |
| B | Magnetic field (usually in the z -direction) |
| ω_n | $(2n+1)\pi/\beta$ |
| Ω | Thermodynamic potential for the interacting system |
| Ω_0 | Thermodynamic potential for the non-interacting system. |
| M | 1) Magnetization, or 2) Ion mass of the host in a dilute alloy. |
| μ | Chemical potential of the system of electrons. |
| ω_c | (eB/mc) ; cyclotron resonance frequency. |
| c | 1) velocity of light or 2) concentration of the alloy. |
| g | electron band g factor (also used for variable coupling constant in ch. II) |
| \bar{g} | Screened electron-phonon coupling constant. |
| μ_B | $(e \hbar/2mc)$; the Bohr magneton. |