THEORY OF TRANSITION ELEMENT SUPERCONDUCTORS

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ABSTRACT

THEORY OF TRANSITION ELEMENT SUPERCONDUCTORS

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A theoretical expression for electron-phonon coupling is derived and then used in an attempt to explain differences in superconducting transition temperatures for groups VB and VIB transition metals.

The bare ionic potential, based upon the Herman-Skillman atomic structure calculations, is used to determine unscreened coupling. Screening is then calculated using the Bardeen self-consistent field method modified for exchange. The net result is an expression for the screened electron-phonon coupling, $g_{K\,K'}$, exhibiting a positive dependence upon the electronic density of states at the Fermi level. Such a dependence is due entirely to exchange and is thought to stem from the preference of conduction electrons to group between nearest neighbors in some resonant structure remnant of atomic "d"-electrons.

A suitable computer program is developed to determine the product of coupling times phonon density of states as a function of phonon frequency, $\alpha^2(\omega)F(\omega)$. The method first uses interatomic force constants to determine the phonon density of states, $F(\omega)$, via the Born-von Karman method. The expression for screened electron-phonon coupling is then incorporated to include umklapp as well as normal scattering processes. Finally, within the currently accepted theory of superconductivity, $\alpha^2(\omega)F(\omega)$ is used to determine an expression for the superconducting transition temperature of tantalum and tungsten.

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CHAPTER I

INTRODUCTION

The first successful microscopic theory of superconductivity was presented by Bardeen, Cooper, and Schrieffer (B.C.S.) in 1957[1] and then later refined into a more elegant and accepted form by Valatin[2] and Bogoliubov[3]. In simplest terms, the theory assumes attractive Cooper[4] electrons forming pairs of opposite momentum and spin which reside in a condensed ground state $|\psi_o\rangle$. A reduced hamiltonian ($H_{red.}$) which considers only the electron pairs is used in conjunction with a parameterized trial ground state wavefunction subject to the constraint that the expectation value of the total number of particles is some fixed number N_o. Let $C^{\dagger}_{k\uparrow}$ and $C_{k\downarrow}$ be creation and annihilation operators for electrons in state k(spin 1/2) and state -k(spin -1/2) respectively.

Then
$$H_{red.} = \sum_{k,s} \epsilon_k C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} C_{-k\downarrow} C_{k\uparrow}$$

$$+\sum_{k,k'} \langle k',-k'|V|k,-k\rangle C^\dagger_{k'\uparrow} C^\dagger_{-k'\downarrow} C_{-k\downarrow} C_{k\uparrow} \qquad 1$$

and

$$\langle \psi_0 | \sum_{k,s} C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} C_{-k\downarrow} C_{k\uparrow} | \psi_0 \rangle = N_0 \qquad 2$$

with

$$|\psi_0\rangle = \prod_k \frac{1 + \lambda_k C^\dagger_k}{\sqrt{1+\lambda_k^2}} |\psi_{VAC.}\rangle . \qquad 3$$

The parameter λ_k in the ground state wavefunction is then determined by normal variational methods for a minimum ground state free energy (see Schrieffer^5). The key results are that the pairing phenomenonis effective within a small range of energies of approximately $2\hbar\omega_D$ (ω_D = Debye frequency) about the Fermi energy and that quasiparticle excitations from the ground state always have an energy greater than or equal to an energy gap Δ. The B.C.S. result for Δ is, in the weak coupling limit (small V),

$$\Delta \cong 2\hbar\omega_D e^{-1/N(0)V} \qquad 4$$

$$2\Delta \cong 3.5 k_B T_c \qquad 5$$

where N(o) is the density of electronic states at the Fermi energy and V is an effective pairing potential acting only within the range of energies about the Fermi level where pairing is approximately assumed to exist. Although the B.C.S. theory was highly successful in predicting qualitative features of superconductors, it soon became apparent that a more powerful theory was due. One had to consider the retarded nature of the electron-phonon interaction and the screened coulomb repulsion between electrons before serious attempts could be made to calculate quantitative properties of superconductors from first principles.

A particularly useful feature of the B.C.S. theory is the isotope effect. If one considers the isotopes of any particular element, each arranged in its own lattice, the normal frequencies of vibration will be $\omega^2 \propto k/M$ in the harmonic approximation where M is the mass of the isotope in the lattice in question and k is an effective spring constant common to all the isotopes of that particular element. Since the transition temperature T_c satisfies Eq. 4, then the ratio of the transition temperatures between any two isotopes of a given element is

$$\frac{T_{c_1}}{T_{c_2}} = \sqrt{\frac{M_2}{M_1}} \quad . \tag{6}$$

This important result is known as the isotope effect. Although it does not include the effects of mutual coulomb repulsion between pairs, it is supported quite well by the simple metals including such strong coupled superconductors (V large) as lead and mercury. However, transition metal superconductors are a different story altogether. They seem to exhibit little or no isotope effect and agreement exists in too few cases to produce any firm conclusions. The results of measurements of the superconducting transition temperatures of various isotopes is shown in table 1 where $T_C \propto M^{-\beta}$ [6]. It would seem that for the transition metals, the B.C.S. theory fails because either the electron pairing potential is not phonon mediated but possibly due to some overscreening by nonsuperconducting electrons in different bands as suggested by several authors[7] or that some electronic mechanism, intermediate to the superconducting electrons and the ions, serves to alter the bare electron-phonon coupling constant in ways more complex than previously described.

Not long after the advent of the B.C.S. theory, theoreticians attempted to apply Green function methods to the superconducting many body problem. Their goal was to develop a theory that would predict the superconducting properties of metallic superconductors from the most basic properties of the metals themselves. Ordinary Green

Table 1. Isotope effect (experimental) for some simple and transition metals.*

Simple		Transition	
Metal	β	Metal	β
Pb	0.48	Os	0.21
Hg	0.50	Ru	0
Sn	0.51	Mo	0.33
Tl	0.49		
Zn	0.50		
Cd	0.40		

* The quantity β is defined with $T_c \sim M^{-\beta}$.

functions soon met with failure due to infinities resulting from summing over certain Feynman diagrams of a given order. The culprits are those diagrams where two electrons of opposite momenta and spin repeatedly scatter against each other. These difficulties were soon surmounted, however, with the introduction of "anomalous propagators" (see Gorkov[8]) which destroy and create Cooper[4] pairs in the ground state. The entire Green function problem was reformulated into a matrix form (Nambu[9]) and was successfully applied by Eliashberg[10] to the problem of strong coupled superconductors.

Strong coupling was particularly troublesome because a large electron-phonon coupling constant would tend to produce such energetic quasiparticle excitations that the resulting lifetimes would be considerably shortened (because of increased available phase space for their decay) to the point where the width (due to uncertainty considerations) of the quasiparticle levels is comparable to the energy of the excitations themselves. The problem was acute until an important result by Migdal[11] was applied by Eliashberg[10] yielding a set of coupled integral equations which form the basis of the theory as it stands today. Important coulomb effects were soon incorporated[12] giving a set of equations (known as the Eliashberg gap equations) which should enable one to calculate the superconducting properties of metals and semiconductors to a relatively high degree of accuracy. These equations form a vital part of this research and, therefore, will be developed in detail later.

Use of the Eliashberg equations to find the superconducting transition temperature T_c was successfully applied to aluminum, sodium, and potassium by Carbotte and Dynes[13]. Essentially, they began by using the Heine-Abarenkov form of the electron-ion pseudopotential[14] from which they could obtain the electron-phonon coupling constant. The necessary phonon characteristics were represented through the use of a Born-von Karman force constant fit to phonon dispersion data in the high crystalline symmetry directions where the number of nearest neighbors considered depended upon the complexity of the phonon dispersion curves for the superconductor in question. The Eliashberg equations were then solved self consistently on a computer yielding results that were quite successful. The transition temperature for both nonsuperconducting sodium and potassium was determined to be less than 10^{-5} °K. For aluminum, the predicted transition temperature differed by less than 10% from the experimental value. In addition, the first strong coupled superconductor to be investigated using the Eliashberg equations was lead which has the pecularities as described earlier. Experimental results for lead strongly support the Eliashberg form as opposed to previous models. Finally, little or no progress has been made in determining the superconducting properties of transition metals from first principles. Their electronic band structure is of such complexity that it is difficult, if not impossible, to make use of pseudopotential methods to determine values of electron-phonon coupling.

If the Eliashberg equations are considered a truly accurate set of solutions to the problem of superconductivity and if superconducting properties can be accurately measured, then it would be logical to ask if these equations could be applied in reverse to determine some of the more elusive properties of solids from their superconducting properties. Such a problem was undertaken by McMillan[15] who applied it to a variety of materials including transition metal superconductors and their alloys. The primary objectives were an empirical electron-phonon coupling constant λ and a coulomb coupling constant μ^* as defined by Morel and Anderson[16]. From these empirical constants the quantity $\langle G^2 \rangle$ (the average squared electronic transition matrix element[17] was found for several transition metal superconductors. All of this was accomplished as follows. The average electron-phonon coupling $\alpha^2(\omega)$ as a function of frequency and the phonon density of states $F(\omega)$ are determined as the product $\alpha^2(\omega)F(\omega)$ directly through the insertion of experimentally determined superconducting properties into the Eliashberg equations. Then the quantity $\langle G^2\rangle$ is:

$$\langle G^2\rangle = \frac{\lambda M}{N(0)}\langle\omega^2\rangle \tag{7}$$

where $$\lambda = 2\int \frac{d\omega\,\alpha^2(\omega)F(\omega)}{\omega} \tag{8}$$

and $$\langle\omega^2\rangle = \frac{\int d\omega\,\alpha^2(\omega)F(\omega)\,\omega}{\int \frac{d\omega\,\alpha^2(\omega)F(\omega)}{\omega}}\,. \tag{9}$$

The results are summarized in table 2. In this scheme McMillan has demonstrated that, for group V and VI B.C.C. transition metals (except magnetic chromium), the factor $N(0)\langle G^2\rangle$ remains essentially constant and that T_c depends upon $M\langle\omega^2\rangle$ (the stiffness of the lattice). These results are uncommon and, as he pointed out, no satisfactory theoretical explanation has been given for such phenomena.

The present theory of superconductivity seems to be satisfactory with the possible exception of the transition

Table 2. Summary of physical parameters influencing superconductivity[15].

Metal	T_c (°K)	θ_D (°K)	γ (mJ/mole°K^2)	N(0) (states/eVatom)	$[\omega^2]^{1/2}$	$[G^2]$ (eV^2/Å^2)	N(0)$[G^2]$ (eV/Å^2)
V	5.30	399	9.9	1.31	290	3.5	4.6
Nb	9.22	277	7.8	0.91	230	7.9	7.2
Ta	4.48	258	6.0	0.77	170	7.9	6.1
Mo	0.92	460	1.83	0.275	310	24.6	6.8
W	0.012	390	0.90	0.148	250	42.5	6.3
Al	1.16	428	1.35	0.206	330	9.7	2.0
In	3.40	112	1.69	0.21	110	8.4	1.76
Pb	7.19	105	3.00	0.30	75	7.8	2.34

metals. These metals can be among the best superconductors and, when properly alloyed, the transition temperature and critical field can be greatly increased (i.e. Nb_3 Sn and V_3Si) which seems to indicate that physical features which give rise to superconductivity are very sensitive to the electronic structure in the case of Nb and V. If one plots the transition temperature T_c versus the number of valence electrons per atom for transition metals and compares it with a similar plot for simple metals, as was done by Matthias[18], (Figure 1), there appears to be little agreement as to how T_c varies with the number of valence electrons per atom. This certainly suggests that, as in many other phenomena, transition metal superconductors must require a modified or perhaps totally different treatment than was used for the case of simple metals. In fact, if one compares the transition temperatures of the group V transition metals with those of group VI transition metals, it becomes apparent that, with the addition of one more non-core electron per atom, the excellent superconducting properties of group V are lost in group VI. Assuming that the theory of superconductivity is correct, it is then logical to try to find a means to determine the degree of electron-phonon coupling and the best value for the density of states (including only those electrons that can take part in pair-

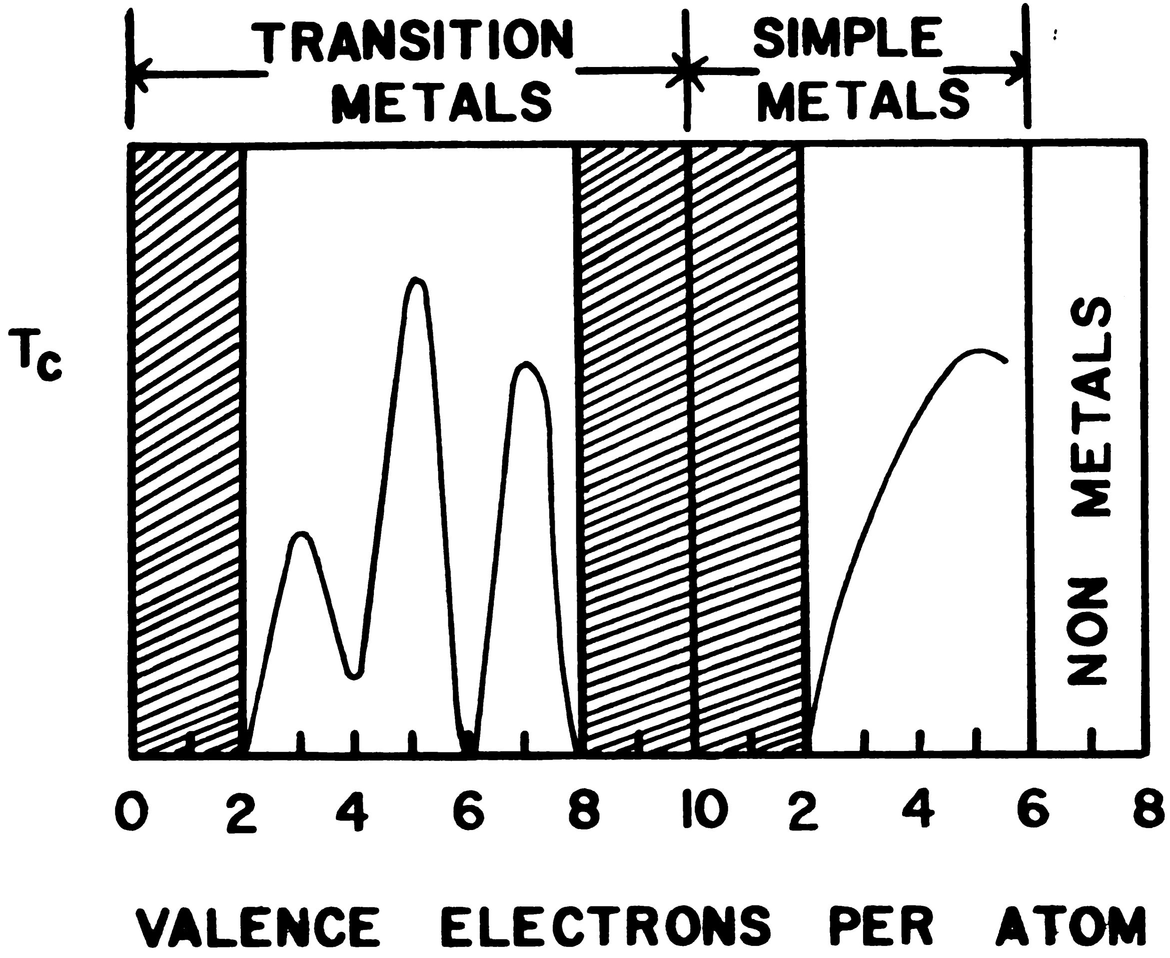


Figure 1. Qualitative behavior of superconducting transition temperatures through the periodic system.

ing) for these two groups. It certainly would not be unreasonable to suppose that not all of the remnants of the s and d atomic states are itinerant. Perhaps a sizable fraction are not available for pairing but do act as an intermediate device to enhance coupling between the paired electrons and the ions. This would most likely reduce the density of available states but, at the same time, could substantially increase the effective electron-phonon interaction. Such a concept is worthy of consideration and, therefore, will be explored in as much detail as present knowledge of the group V and VI transition metals will allow.

CHAPTER II

THE THEORY

This problem is primarily concerned with the electronic structure of the group V and group VI transition metals. As completely free atoms, transition elements are characterized by two partially filled atomic subshells (3d4s, 4d5s, or 5d6s) as opposed to the usual <u>one</u> (or completely filled shells as in the case of the inert gases). The number of electrons residing in both the s and d subshells determines the chemical and metallurgical characteristics of the element in question. For groups V and VI, the atomic configurations are:

group V	group VI
$V-3d^3 4s^2$	$Cr-3d^5 4s$
$Nb-4d^4 5s$	$Mo-4d^5 5s$
$Ta-5d^3 6s^2$	$W-5d^4 6s^2$

The objective is to determine how these electrons in partially filled subshells (valence electrons) interact with valence electrons of adjacent atoms in a metallic solid. It is often stated that the unfilled s and d subshells transform into overlapping s and d bands in the solid state. Moreover, a frequent assumption is that the relative proportion of electrons in each of these bands is the same as it was for the partially filled atomic subshells. A more realistic viewpoint, however, is one proposed by several authorities[19,20] in this area which is that the valence electrons collect into two fairly distinct groups. One such group is quite localized and may possibly be represented by some linear combination of the former d orbital wavefunctions. The second group would be an itinerant conduction-like band which could probably be represented by plane waves properly orthogonalized to both core states and the localized states of the first group. It seems plausible that these two bands overlap with the localized band being the narrower of the two. Moreover, the number of electrons per atom residing in each of these bands would, in all likelihood, not be in the same proportion as the relative numbers of electrons in the s and d atomic subshells respectively. Such are the foundations to be later utilized in setting up an electronic model of the group V and VI transition metals.

If one is to base a model on the concept of two overlapping bands where one is localized and the other itinerant and conduction-like, then it is fruitful at first to investigate how such a configuration might affect the pairing interaction in superconductors. The conditions for pairing are most favorable with a strong electron-phonon coupling constant and a high available electronic density of states at the Fermi surface. The question then arises as to whether all of the valence electrons are available for pairing. Perhaps either the more localized electrons or the conduction electrons do not take part in the pairing process at all and hence one must use a density of states that accurately reflects this reduction of available electronic states. Certainly, then, if a given proportion of the valence electrons do not contribute to the pairing process, transition metal superconductivity may be enhanced through a mechanism other than a high electronic density of states. Another possibility would be to examine how these non-superconducting valence electrons might tend to modify ion (phonon) coupling to the superconducting electrons. If this modified coupling were quite sensitive to the number of electrons in localized bands, then the difference of a valence electron per atom between transition groups V and VI could account for the gross contrast between their ability to superconduct provided the extra electron in group VI were in the localized d band.

The model to be used will be one in which n_d valence electrons per atom reside in localized d-like band states and n_c valence electrons per atom form an itinerant conduction band. The question naturally arises as to which band

contains the superconducting electron pairs. In the past, it has been quite customary to consider the itinerant electrons as those available for pairing [21,22]. The localized states are then usually treated as either intermediate states for electron pair scattering by the lattice ions or as states acting directly between the pairs by providing an additional attractive coupling mechanism. McMillan[15] seems to avoid this question altogether when he uses a density of states based upon the electronic specific heat γ . Although the argument for d-like electrons over-screening the conduction electrons would enhance superconductivity, it makes little sense to consider electrons with a supposedly high effective mass as capable of screening the effectively lighter conduction electrons. However, it would not suffice to say that electrons with high effective mass cannot be screening agents in the case of the ions due to the fact that they are also strongly coupled (source of high effective mass). Whether or not screening of one band by a second could enhance the electron-ion interaction of the first should be analyzed. These arguments give rise to two possibilities:

(1) The conduction band electrons form superconducting pairs. The d-band electrons screen the motion of the ions in such a way so as to enhance electron-phonon coupling in group V and diminish it in group VI. The difference in

superconducting properties between groups V and VI is attributed to the difference of one electron per atom in the d-band.

(2) The d-band electrons form superconducting pairs. The conduction band electrons serve as a screening mechanism to alter electron-phonon coupling and reduce the effective coulomb repulsion between d band electrons. The high density of states of the group V d band at the Fermi level greatly assists superconductivity whereas a small density of states in group VI all but destroys it. Again, there is a difference of one electron per atom in the d bands of group V and group VI.

One of the most crucial portions of the model will be the structure of the localized electrons. One must know their density of states distribution, energies, and, if possible, their wavefunctions. Unlike core electrons, the localized electrons cannot be associated solely with a particular ion within the crystal. The characteristic that distinguishes them from conduction electrons is that their distribution varies grossly within the structure of the unit cell. Localized electrons will tend to bunch up mainly between nearest neighbors and next nearest neighbors respectively. Such electrons should be sensitive to the motion of the ions even though they cannot be associated solely with any one particular lattice site. Since both group V and group VI transition metals have BCC crystal structure, it is best to examine splitting of d-orbital wavefunctions in a cubic field before attempting to use them in constructing localized band states. Basis functions from which the localized states can be formed are as follows:

$$XY=\sqrt{2\pi/15}\left\{Y_2^{2}(\theta,\phi)-Y_2^{-2}(\theta,\phi)\right\}$$

$$YZ=\sqrt{2\pi/15}\left\{Y_2^{-1}(\theta,\phi)+Y_2^{1}(\theta,\phi)\right\}$$

$$ZX=\sqrt{2\pi/15}\left\{Y_2^{-1}(\theta,\phi)-Y_2^{1}(\theta,\phi)\right\}$$

$$X^2-Y^2=\sqrt{8\pi/15}\left\{Y_2^{2}(\theta,\phi)+Y_2^{-2}(\theta,\phi)\right\}$$

$$3Z^2-R^2=\sqrt{16\pi/15}\left\{Y_2^{0}(\theta,\phi)\right\}$$

where $Y_2(\theta,\phi)$ are the orthonormal spherical harmonics forming a basis for the angular part of atomic d wavefunctions. These new basis functions are all mutually orthogonal and therefore must span the same space as Y_2 . The purpose of the particular basis becomes quite clear when one examines the full cubic group O_h,(Table 3) . The functions X^2-Y^2 and $3Z^2-R^2$ form a basis for the two diminsional representation E_g and XY, YZ, and ZX form a basis for the three diminsional represen-

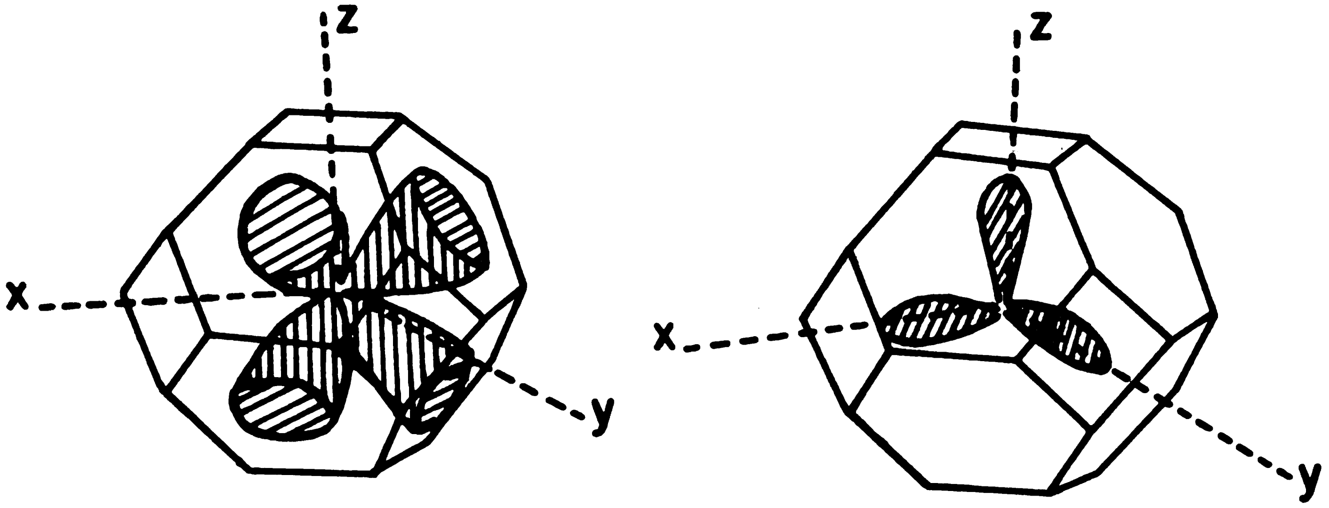
Table 3. Character table of the cubic group O.*

	Class	E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$
Basis	Representation					
R^2	A_1	1	1	1	1	1
$X^2-Y^2, 3Z^2-R^2$	E	2	-1	2	0	0
	A_2	1	1	1	-1	-1
X,Y,Z	T_1	3	0	-1	-1	1
XY,YZ,ZX	T_2	3	0	-1	1	-1

*The full cubic group $O_h = O \otimes I$ where I is the inversion group[23].

tation T_{2g} . This means that under spatial operations which preserve the symmetry of the full cubic group, these basis functions do not mix but transform only into linear combinations of the members belonging to their own particular basis. For small cubic crystal fields, the five-fold degenerate atomic d-levels would be split into a doubly degenerate E_g level and triply degenerate T_{2g} level respectively. Stronger cubic fields (as in a crystal) will further split these levels in every atom of the crystal thus forming two distinct bands. These bands are in accord with Fig. 2 showing electronic structures within the BCC primitive cell[24].

These structures as shown in Fig. 2 can be inferred from examination of the angular dependence of XY, YZ, and ZX for the T_{2g} case or X^2-Y^2 and $3Z^2-R^2$ for the E_g case provided that the wavefunctions are formed from proper linear combinations of the basis functions so as to preserve cubic symmetry. Such wavefunctions will be referred to as hybridized T_{2g} or hybridized E_g respectively[24]. Since, in both groups V and VI, there are insufficient valence electrons to fill both T_{2g} and E_g states, it is natural to determine which of these bands would lie at the lowest energy and hence begin filling first. Because it is generally true that nearest neighbor correlations are stronger than next



T_{2g} E_g

Figure 2. Areas of maximum electron density within the B.C.C. primitive cell for electrons having T_{2g} (E_g) group symmetry.

nearest neighbors and so forth for more distant ions, then the states representing correlations between nearest neighbors might be expected to receive electrons at a lower energy than the next nearest neighbor correlated E_g states. Although band structure data is seriously deficient for groups V and VI transition metals, one can investigate the band structure of one particular metal (tungsten) in hope of getting a handle on the essential features of band structures of chemically similar materials. Mattheiss[25] proposes that the band structures of the BCC transition metals (group V and VI) should be quite similar to one another with the Fermi energy being determined from the total number of valence electrons. Upon examination of the theoretical density of states curve as plotted by Mattheiss for tungsten (Fig. 5), there appears to be four fairly distinct peaks with the lower three appearing quite similar. Furthermore, it seems that for up to six valence electrons per atom, the lower portion would provide a sufficient number of states to accomodate all of the valence electrons. Although this problem will be reconsidered later in the discussion of the filling of the bands, it will suffice to say now that the T_{2g} states will be used to represent the localized electrons and the E_g states can be disregarded for the use of six or less valence electrons per atom.

Proper tight binding wavefunctions representing T_{2g} states are:

$$\Lambda^{\delta}_{\underline{K},s}(\underline{r}) = \sqrt{\frac{15}{4\pi N}} \sum_{j} e^{i\underline{K}\cdot\underline{r}_j} \phi_{\delta}(\underline{r}-\underline{r}_j)\, \chi_s(\underline{r}) \qquad 1$$

where the sum over j is over the entire lattice and

$$\phi_1 = f(r)\, XY, \; \phi_2 = f(r)\, YZ \quad \text{and} \quad \phi_3 = f(r)\, ZX . \qquad 2$$

The convergence factor $f(r)$ satisfies the normalization condition that $\int_0^\infty f^2(r)\, r^6 dr = 1$ and is best guessed at from the atomic d-electron radial wavefunctions[26] or the band structure itself. If $f(r)$ is normalized as it is here, then these wavefunctions represent a continuum of states in k-space and, hence, must be used with an electronic density of states. Later it may become necessary to modify the spin density of $\Lambda^{\delta}_{\underline{K},s}(\underline{r})$ to reflect the occurance of antiferromagnetic structure in this band. Such a modification can be included in the spinor factor $\chi_s(\underline{r})$ which may be set to vary spatially from spin up to spin down with a period one half of that of the lattice.

Representation of the conduction states should be much simpler. For one thing, the density of these electrons should not vary grossly within the unit cell since they are free electron like and hence are most easily represented by some variety of plane wave. Ordinary plane waves would suffice but should require that a large number of them be used in order to cope with strongly varying potentials throughout the crystal. On the other hand, augmented plane waves (APW) are particularly advantageous in the sense that they are most frequently used in band structure calculations making it easier to apply the results of such calculations to this particular investigation. Orthogonal plane waves (OPW) offer a third alternative which should be most compatible with using tight binding functions to represent the localized states.

$$\psi_{\underline{k},s}(\underline{r}) = \left\{ \frac{e^{i\underline{k}\cdot\underline{r}}}{\sqrt{N}} - \frac{1}{\sqrt{N}} \sum_{\delta} \langle \Lambda^{\delta}_{k}(\underline{r}') | e^{i\underline{k}\cdot\underline{r}'} \rangle \Lambda^{\delta}_{k}(\underline{r}) \right\} \chi_{s}(\underline{r}) \tag{3}$$

For $\delta = 1, 2,$ or 3, Λ represents a localized d state whereas other values of δ imply core states. Again, it may become necessary to include a spatially dependent spinor factor $\chi_{s}(\underline{r})$ if antiferromagnetic effects appear to become important.

Up until now, the important parameters n_c and n_d (the numbers of conduction electrons and localized electrons per atom respectively) have remained unspecified. Since the

localized T_{2g} electrons are nearest neighbor correlated, they should contribute substantially to lattice bonding. The reason is that there exists a critical atomic separation R_c as noted by Goodenough[24] such that when nearest neighbor separations are less than R_c, correlated electrons T_{2g} should exhibit a net bonding. Although it is usually difficult to predict just how many the localized d-band would accept for optimum bonding, some relevant information can be gained through examination of the magnetic properties of the system. Slater[27] has proposed the possibility of spin correlations between nearest neighbors. Such correlations would be antiferromagnetic if the band were half or less filled and ferromagnetic if it were more than half filled. Moreover, any spin correlations would tend to split the T_{2g} band into a bonding and an antibonding part with each capable of accepting three electrons. The bonding states would naturally be lower and hence transition metals with nearly half-filled T_{2g} bands would be among the strongest structurally, i.e. groups V and VI. It is interesting to note that the only ordered magnetic material in groups V and VI is chromium having a net antiferromagnetic moment of 0.4 Bohr magnetron per atom. As pointed out by Jensen and Suhl[28], even weak magnetic ordering can seriously disrupt superconductivity and, although the coexistance of ferromagnetism and the superconducting state has been predicted[29], it has yet to be observed. All of this means that it may not be strictly valid to say that chromium is a poor superconductor for the same reason as molybdenum and tungsten. More than likely the processes which tend to discourage superconductivity in molybdenum and tungsten are present in chromium so that it will still be instructive to consider it along with the others. Slater[27] seems to justify such unique behavior of chromium by supposing that the Fermi level of the itinerant electrons does not lie within the gap of the split T_{2g} band. Hence, no net reduction in energy could be realized in the first place by splitting of the T_{2g} states since an equal number of electrons would both raise and lower their energy upon appearance of the gap producing no net energy change required for stabilization. Additional light is shed on this problem by the density of states calculation for tungsten (Fig. 5). In this case it is quite apparent that the T_{2g} states are probably no more than half-filled providing that there are approximately the same number of itinerant electrons as localized ones. In fact, it is important to observe at this point, if group V had two T_{2g} electrons per atom and group VI had three, then changing from a partially filled bonding half band to a fu

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full one may be just the mechanism that effects electron-phonon coupling and the electronic density of states in such a way as to diminish superconductivity in group VI.

As for the itinerant electrons, strong arguments for three such electrons per atom are presented by Goodenough[25]. These range from observation of the forbidden soft x-ray transitions (indicating a strong admixture of p-states in this band) to experiments in solid solubility. In any event, when it is assumed that there are three itenerent electrons per atom in groups V and VI, the localized T_{2g} states cannot be more than half filled. Moreover, three electrons per atom would still result in a more than adequate density of available itinerant conduction states to form a strongly superconducting band in the case of group V.

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CHAPTER III

THE GAP EQUATIONS

The key to successful quantitative investigation of superconducting phenomena is to realize that the energy difference associated with the superconducting phase change is miniscule (about 10^{-8}eV per conduction electron). With the methods presently available it would be impossible to predict superconductivity from a first principles calculation. Thus it is necessary to devise a model which treats only the subtle interactions leading to this phenomenon. To accomplish this one must already have at hand the correct qualitative picture which assumes the existence of electron pairs[4] whose momenta are correlated as the result of a net attractive electron-phonon interaction[36]. Hence, when writing down an interaction Hamiltonian, one must include only the mechanisms specifically leading to superconductivity whilst all other interaction terms can only be included in the unperturbed Hamiltonian. An additional consideration must be included. This is that the electron pairs are "condensed" into the ground state (excited pairs are ruled out in metals as having energies very much higher than observed for excitations in superconductors). Thus, in the unpaired remainder of the system being treated by many-body techniques, provision must be made for the effect of pairs entering and leaving the condensed state. Moreover, in the unpaired system the total number of particles will not be a quantum number but the average number for such a system at equilibrium will, of course, be the expectation value of the number operator. This allows terms in the Hamiltonian which do not conserve the total number of particles, i.e. those operators that create or destroy one electron pair.

Before applying the Green function technique, the Nambu[30] formalism will be specified. This technique involves essentially a matrix Green function whose off diagonal elements represent Gorkov[11] anomalous propagators which transfer electron pairs in and out of the condensate and has become the more or less standard form of notation in the theory as it stands today. In order to find the exact solution from Dyson's equation one uses the full Hamiltonian which is:

H= Σ (Bloch energies of electrons) + Σ (energies of phonons) + Σ (interactions between electrons) + Σ (interactions between electrons and phonons) + (other terms, i.e. phonon-phonon interactions, etc.)

Or, in the notation of second quantitization

$$H=\sum_{\underline{k},s}\epsilon_{\underline{k}}C^{\dagger}_{\underline{k},s}C_{\underline{k},s}+\sum_{\underline{q},\alpha}\hbar\,\omega_{\underline{q},\alpha}a^{\dagger}_{\underline{q},\alpha}a_{\underline{q},\alpha}$$

$$+\sum_{\underline{k},\underline{k}',s,\alpha}\bar{g}_{\underline{k},\underline{k}',\alpha}\left(a^{\dagger}_{-\underline{q},\alpha}+a_{\underline{q},\alpha}\right)C^{\dagger}_{\underline{k}',s}C_{\underline{k},s}$$

$$+\frac{1}{2}\sum_{\underline{k},\underline{k}',\underline{l},s,s'}\langle\underline{k}-\underline{l}|\langle\underline{k}'+\underline{l}|V|\underline{k}'\rangle|\underline{k}\rangle C^{\dagger}_{\underline{k}-\underline{l},s}C^{\dagger}_{\underline{k}'+\underline{l},s'}C_{\underline{k}',s'}C_{\underline{k},s}+\cdots \qquad 1$$

where $\epsilon_{\underline{k}}$ are the Bloch energies relative to the Fermi level and V is the screened coulomb interaction as a function of the distance between two electrons. Using Nambu's notation, define new field operators in terms of column and row matricies.

$$\Psi_{\underline{k}}=\begin{pmatrix}C_{\underline{k}\uparrow}\\ C_{-\underline{k}\downarrow}\end{pmatrix}\quad,\quad \Psi^{\dagger}_{\underline{k}}=\begin{pmatrix}C^{\dagger}_{\underline{k}\uparrow} & C_{-\underline{k}\downarrow}\end{pmatrix} \qquad 2$$

where the arrows ↑ and ↓ denote spin up and down respectively. Next using $\sigma_{z}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, express the Hamiltonian in terms of these field operators noting that the spin is handled automatically.

Thus, $\sum_{\underline{k},s}\epsilon_{\underline{k}}C^{\dagger}_{\underline{k},s}C_{\underline{k},s}=\sum_{\underline{k}}\epsilon_{\underline{k}}\left(C^{\dagger}_{\underline{k},\uparrow}C_{\underline{k},\uparrow}+C^{\dagger}_{\underline{k},\downarrow}C_{\underline{k},\downarrow}\right)$

$$=\sum_{\underline{k}}\epsilon_{\underline{k}}\left(C^{\dagger}_{\underline{k}\uparrow}C_{\underline{k}\uparrow}+C_{-\underline{k}\downarrow}C^{\dagger}_{-\underline{k}\downarrow}+1\right)=\sum_{\underline{k}}\epsilon_{\underline{k}}\,\Psi_{\underline{k}}\,\sigma_z\,\Psi_{\underline{k}}+\sum_{\underline{k}}\epsilon_{\underline{k}}\quad,$$

$$\sum_{k,k',s,\alpha}\bar{g}_{\underline{k},\underline{k}',\alpha}\left(a^{\dagger}_{-\underline{q},\alpha}+a_{\underline{q},\alpha}\right)C^{\dagger}_{\underline{k}',s}C_{\underline{k},s}$$

$$=\sum_{\underline{k},\underline{k}',\alpha}\bar{g}_{\underline{k},\underline{k}',\alpha}\left(a^{\dagger}_{-\underline{q},\alpha}+a_{\underline{q},\alpha}\right)\left(C^{\dagger}_{\underline{k}'\uparrow}C_{\underline{k}\uparrow}+C^{\dagger}_{\underline{k}'\downarrow}C_{\underline{k}\downarrow}\right)$$

$$=\sum_{\underline{k},\underline{k}',\alpha}\bar{g}_{\underline{k},\underline{k}',\alpha}\left(a^{\dagger}_{-\underline{q},\alpha}+a_{\underline{q},\alpha}\right)\Psi^{\dagger}_{\underline{k}'}\,\sigma_z\,\Psi_{\underline{k}}\quad,$$

$$\frac{1}{2}\sum_{\underline{k},\underline{k}',s,s',\underline{l}}\langle\underline{k}-\underline{l}|\langle\underline{k}'+\underline{l}|V|\underline{k}'\rangle|\underline{k}\rangle C^{\dagger}_{\underline{k}-\underline{l},s}C^{\dagger}_{\underline{k}'+\underline{l},s}C_{\underline{k}',s}C_{\underline{k},s}$$

$$=\frac{1}{2}\sum_{\underline{k},\underline{k}',\underline{l}}\langle\underline{k}-\underline{l}|\langle\underline{k}'+\underline{l}|V|\underline{k}'\rangle|\underline{k}\rangle\Big\{C^{\dagger}_{\underline{k}-\underline{l},\uparrow}C^{\dagger}_{\underline{k}'+\underline{l},\uparrow}C_{\underline{k}',\uparrow}C_{\underline{k},\uparrow}+$$

$$C^{\dagger}_{\underline{k}-\underline{l},\uparrow}C^{\dagger}_{\underline{k}'+\underline{l},\downarrow}C_{\underline{k}'\downarrow}C_{\underline{k}\uparrow}+C^{\dagger}_{\underline{k}-\underline{l},\downarrow}C^{\dagger}_{\underline{k}'+\underline{l},\uparrow}C_{\underline{k}'\uparrow}C_{\underline{k}\downarrow}+C^{\dagger}_{\underline{k}-\underline{l},\downarrow}C^{\dagger}_{\underline{k}'+\underline{l},\downarrow}C_{\underline{k}'\downarrow}C_{\underline{k}\downarrow}\Big\}$$

$$=\frac{1}{2}\sum_{\underline{k},\underline{k}',\underline{l}}\langle\underline{k}-\underline{l}|\langle\underline{k}'+\underline{l}|V|\underline{k}'\rangle|\underline{k}\rangle\left(\Psi^{\dagger}_{\underline{k}-\underline{l}}\,\sigma_z\,\Psi_{\underline{k}}\right)\left(\Psi_{\underline{k}'+\underline{l}}\,\sigma_z\,\Psi_{\underline{k}}\right),$$

or, neglecting the term $\sum_{\underline{k}} \epsilon_{\underline{k}}$ (unneeded in Dyson self energy),

$$H=\sum_{\underline{k}} \epsilon_{\underline{k}} \Psi_{\underline{k}}^{\dagger} \sigma_z \Psi_{\underline{k}} + \sum_{\underline{k},\underline{k}',\alpha} g_{\underline{k},\underline{k}',\alpha}\left(a_{-\underline{q}\alpha}^{\dagger}+a_{\underline{q}\alpha}\right) \Psi_{\underline{k}'}^{\dagger} \sigma_z \Psi_{\underline{k}}$$

$$+\sum_{\underline{q},\alpha} \hbar\omega_{\underline{q}\alpha} a_{\underline{q}\alpha}^{\dagger} a_{\underline{q}\alpha} + \frac{1}{2}\sum_{\underline{k},\underline{k}',\underline{l}} \langle \underline{k}-\underline{l}| \langle \underline{k}'+\underline{l}| V |\underline{k}'\rangle |\underline{k}\rangle \Psi_{\underline{k}-\underline{l}} \sigma_z \Psi_{\underline{k}'} \Psi_{\underline{k}'+\underline{l}} \sigma_z \Psi_{\underline{k}} \qquad 3$$

The following development of the gap equations is largely taken from the finite temperature approach given by Schrieffer, Scalapino, and Wilkins[12] (SSW). The finite temperature phonon propagator is

$$D_{\alpha}(\underline{q},\tau)=-\left\langle T\left\{\phi_{\underline{q}\alpha}(\tau)\, \phi_{\underline{q}\alpha}^{\dagger}(0)\right\}\right\rangle = \frac{1}{\beta}$$

where the brackets < ··· > denote the grand canonical average, T is the Wick time ordering operator[36]

$$\phi_{\underline{q}\alpha}(\tau)=e^{iH\tau}\phi_{\underline{q}\alpha}(0)e^{-iH\tau} = e^{iH\tau}\left(a_{\underline{q}\alpha}+a_{-\underline{q}\alpha}^{\dagger}\right),$$

and $\nu_n = 2\pi n/\beta$. In the Nambu scheme the finite temperature electron propagator becomes

$$G(\underline{k},\tau)=-i\begin{pmatrix} \langle T C_{\underline{k}\uparrow}(\tau) C_{\underline{k}\uparrow}(0)\rangle & \langle T C_{\underline{k}\uparrow}(\tau) C_{-\underline{k}\downarrow}(0)\rangle \\ \langle T C_{-\underline{k}\downarrow}^{\dagger}(\tau) C_{\underline{k}\uparrow}^{\dagger}(0)\rangle & \langle T C_{-\underline{k}\downarrow}^{\dagger}(\tau) C_{-\underline{k}\downarrow}(0)\rangle \end{pmatrix} \qquad 4$$

$$=\begin{pmatrix} G_e(\underline{k},\tau) & F(\underline{k},\tau) \\ F^{\dagger}(\underline{k},\tau) & G_h(\underline{k},\tau) \end{pmatrix} = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau} G(\underline{k}, i\omega_n)$$

where $\omega_n=(2n+1)\pi/\beta$ and $C_{\underline{k}}(\tau)=e^{iH\tau}C_{\underline{k}}(0)e^{-iH\tau}$.

It can be seen that $G(\underline{k},\tau)$ accounts for the condensate with anomalous propagators[11] F^+ and F which create and destroy electron pairs respectively. Dyson's equation is

$$G(\underline{k},i\omega_n)=\left[G_0^{-1}(\underline{k},i\omega_n)-\Sigma(\underline{k},i\omega_n)\right]^{-1} \qquad 5$$

where

$$G_0^{-1}(\underline{k},i\omega_n)=i\omega_n I-\epsilon_{\underline{k}}\,\sigma_z \qquad 6$$

The problem, then, is to determine the self energy $\Sigma(\underline{k},i\omega_n)$. Illustrated with Feynman diagrams, the self energy is shown in Fig. 3. Using the diagram rules given in Mattuck[35], the expression (containing terms up to and including Hartree-Fock) for the self energy is

$$\Sigma(\underline{k},i\omega_n)=-\frac{1}{\beta}\sum_{\underline{k}',n'}\sigma_z\, G(\underline{k}',i\omega_{n'})\,\sigma_z\times$$

$$\left\{\sum_{\alpha}|\bar{g}_{\underline{k}\underline{k}'\alpha}|^2 D_\alpha(\underline{k}-\underline{k}',i\omega_n-i\omega_{n'})+V(\underline{k},\underline{k}')\right\} \qquad 7$$

where $V(\underline{k},\underline{k}')$ is the screened coulomb potential assumed to be independent of ω_n. The spectral representation of the phonon propagator is

$$D_\alpha(\underline{q},i\nu_n)=\frac{1}{2}\int_{-\beta}^{\beta}e^{i\nu_n\tau}D_\alpha(\underline{q},\tau)\,d\tau$$

$$=\mp\frac{i}{2}\int_{-\beta}^{\beta}e^{i\nu_n\tau}\left\langle T\left\{\phi_{\underline{q}\alpha}(\tau)\,\phi^{\dagger}_{\underline{q}\alpha}(0)\right\}\right\rangle d\tau$$

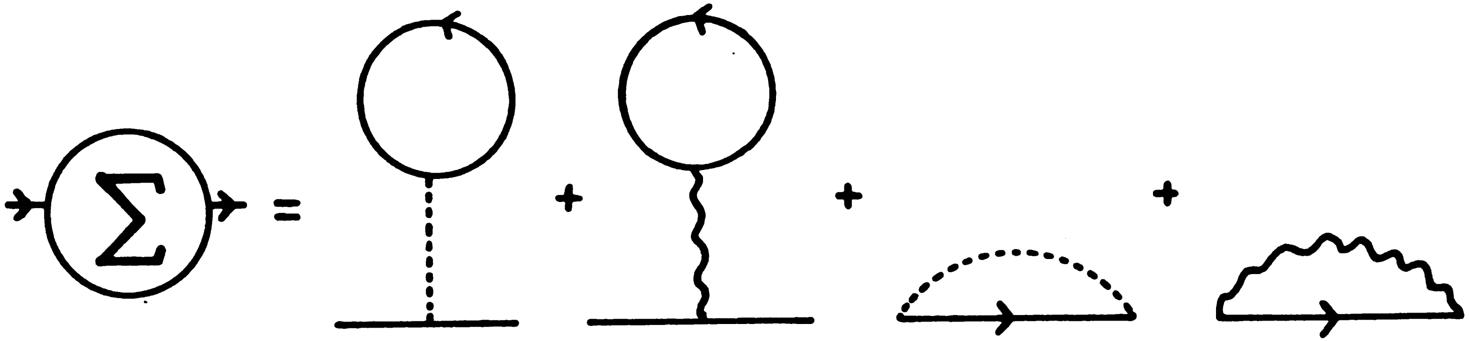

Figure 3. Important diagrams contributing to self energy. Dotted and wavy lines indicate coulomb and phonon processes respectively.

$$= -\frac{i}{2}\int_{-\beta}^{\beta} e^{i\nu_n\tau}\langle\{e^{-iH\tau}\phi_{\underline{q}\alpha}(0)e^{iH\tau}\phi^{\dagger}_{\underline{q}\alpha}(0)\}\rangle d\tau, \quad \tau>0$$

$$= \frac{i}{2}\int_{-\beta}^{\beta} e^{i\nu_n\tau}\langle\{e^{iH\tau}\phi_{\underline{q}\alpha}(0)e^{-iH\tau}\phi^{\dagger}_{\underline{q}\alpha}(0)\}\rangle d\tau, \quad \tau\le 0$$

$$= -\frac{i}{2}\frac{\int_{-\beta}^{\beta} e^{i\nu_n\tau}\sum_i\langle i|e^{-\beta H}e^{-iH\tau}\phi_{\underline{q}\alpha}(0)e^{iH\tau}\phi^{\dagger}_{\underline{q}\alpha}(0)|i\rangle d\tau}{\sum_i\langle i|e^{-\beta H}|i\rangle}, \quad \tau>0$$

$$= \frac{i}{2}\frac{\int_{-\beta}^{\beta} e^{i\nu_n\tau}\sum_i\langle i|e^{-\beta H}e^{iH\tau}\phi_{\underline{q}\alpha}(0)e^{-iH\tau}\phi^{\dagger}_{\underline{q}\alpha}(0)|i\rangle}{\sum_i\langle i|e^{-\beta H}|i\rangle}, \quad \tau\le 0$$

$$= -\frac{i}{2}\frac{\int_{-\beta}^{\beta} e^{i\nu_n\tau}\sum_{ij}\langle i|e^{-\beta H}e^{-iH\tau}\phi_{\underline{q}\alpha}(0)|j\rangle\langle j|e^{iH\tau}\phi_{\underline{q}\alpha}(0)|i\rangle d\tau}{\sum_i\langle i|e^{-\beta H}|i\rangle}, \quad \tau>0$$

$$= \frac{i}{2}\frac{\int_{-\beta}^{\beta} e^{i\nu_n\tau}\sum_{ij}\langle i|e^{-\beta H}e^{iH\tau}\phi_{\underline{q}\alpha}(0)|j\rangle\langle j|e^{-iH\tau}\phi_{\underline{q}\alpha}(0)|i\rangle d\tau}{\sum_i\langle i|e^{-\beta H}|i\rangle}, \quad \tau\le 0$$

$$= \mp\frac{i}{2}\frac{\int_{-\beta}^{\beta} e^{i\nu_n\tau}\sum_{ij} e^{-\beta E_i}e^{\mp(E_i-E_j)\tau}\langle i|\phi_{\underline{q}\alpha}(0)|j\rangle\langle j|\phi^{\dagger}_{\underline{q}\alpha}(0)|i\rangle d\tau}{\sum_i\langle i|e^{-\beta H}|i\rangle}, \quad {}^{(-)\,\tau>0}_{(+)\,\tau\le 0}$$

$$= \frac{i}{2}\frac{\sum_{ij}\left[-\left(e^{i\nu_n\beta-(E_i-E_j)\beta}-1\right)-\left(e^{-i\nu_n\beta-(E_i-E_j)\beta}-1\right)\right.}{\sum_i e^{-\beta E_i}}\times \qquad 8$$

$$\langle i|\phi_{\underline{q}\alpha}(0)|j\rangle\langle j|\phi^{\dagger}_{\underline{q}\alpha}(0)|i\rangle e^{-\beta E_i}$$

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Define the spectral density

$$A_{\alpha}(\underline{k}-\underline{k}',\nu)=\left(\frac{1-e^{\beta\nu}}{2}\right)\frac{\sum_{i,j}|\langle j|\phi_{\underline{q}\alpha}(0)|i\rangle|^{2}\,\delta(\nu-E_j+E_i)}{\sum_i e^{-\beta E_i}} \qquad 9$$

where $\underline{q}=\underline{k}-\underline{k}'$.

Then

$$D(k-k',i\nu_n)=\int_0^{\infty}A_{\alpha}(\underline{k}-\underline{k}',\nu)\left[\frac{1}{i\nu_n-\nu}-\frac{1}{i\nu_n+\nu}\right]d\nu \qquad 10$$

Now substitute Eq. 10 into Eq. 7 and transform the sum over n' into an integral representation using the residues of poles within an infinite contour C to project out terms of the infinite sum, i.e. integrating over the contour will give infinite series of residues of the poles contained within the contour C (see Fig. 4). Functions tanh $\frac{\beta z}{2}$ and $(1+e^{\pm\beta z})^{-1}$, one has the residues for values of $\beta z=\text{odd}\,i\pi$

$$\mathrm{Res}(1+e^{\pm\beta z})=\lim_{z\to\frac{i\pi}{\beta}}\frac{z-i\pi/\beta}{(1+e^{\pm\beta z})}=\frac{\pm e^{\mp i\pi}}{\beta}=\pm\frac{1}{\beta}$$

$$\mathrm{Res}\tanh\frac{\beta z}{2}=\lim_{z\to\frac{i\pi}{\beta}}\frac{e^{\beta z/2}-e^{-\beta z/2}}{(z-\frac{i\pi}{\beta})}\,\frac{(z-i\pi/\beta)}{\beta/2(e^{\beta z/2}-e^{-\beta z/2})}=\frac{2}{\beta}$$

Now, making use of these residues, let $i\omega_{n'}\to z$ to get

$$\Sigma(\underline{k},i\omega_n)=-\frac{1}{2\pi i}\sum_{\underline{k}'}\sigma_z\int_C G(\underline{k}',z)\sigma_z\Big[\sum_{\infty}|\bar{g}_{\underline{k}\underline{k}'\alpha}|^2\int_0^{\infty}A_{\alpha}(\underline{k}-\underline{k}',\nu)\times$$

$$\left\{\frac{1}{(i\omega_n-z-\nu)(1+e^{-\beta z})}+\frac{1}{(i\omega_n-z+\nu)(1+e^{\beta z})}\right\}d\nu+\frac{V(k,k')}{2}\tanh\frac{\beta z}{2}\Big]dz \qquad 11$$

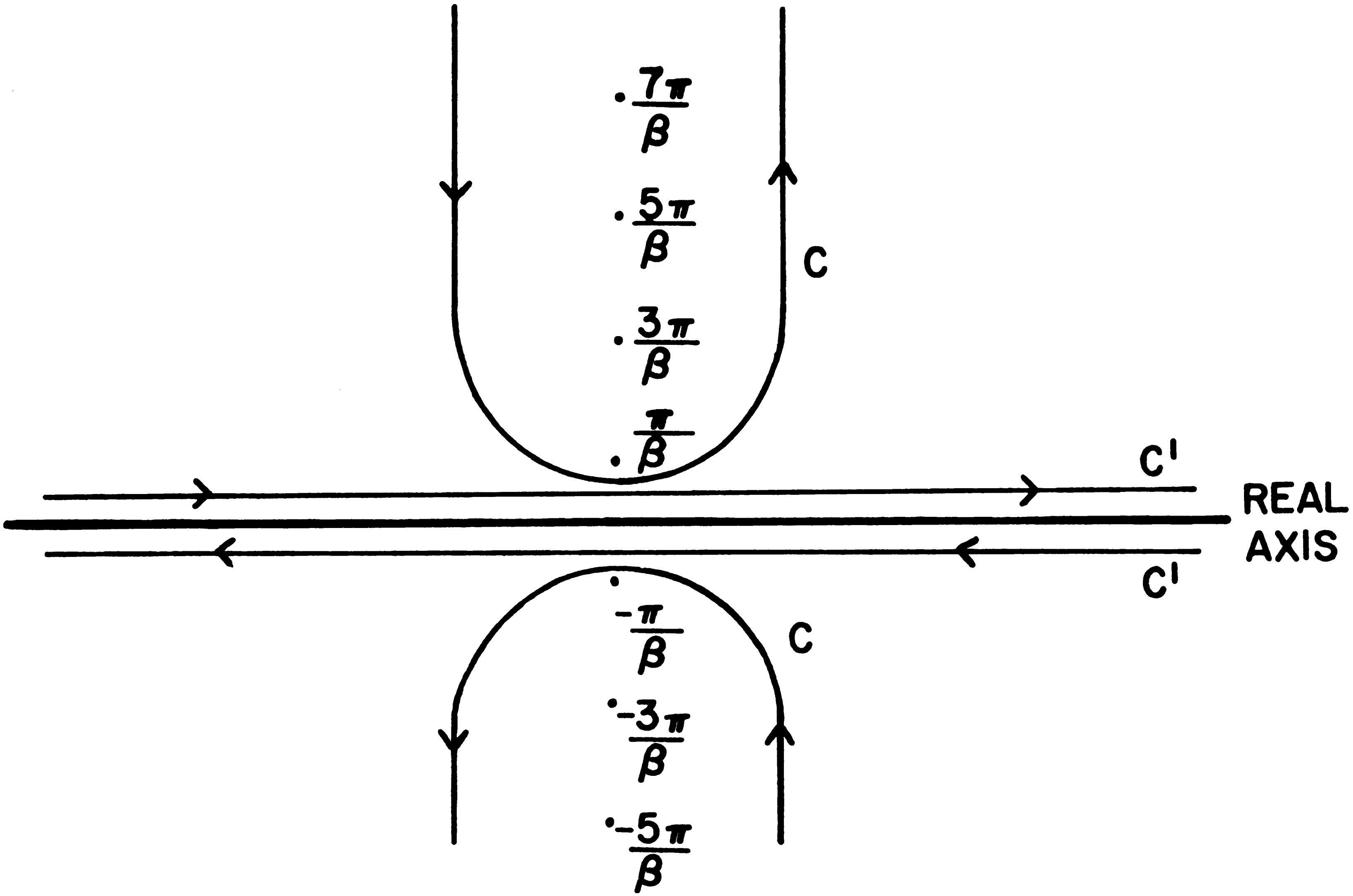

Figure 4. Contours in complex plane showing some poles at odd Π/β.

When the contour is deformed to C', two additional poles must be included whose residues are

$$\mathrm{Res}\frac{G(\underline{k}',z)}{(i\omega_n-z\pm\nu)(1+e^{\pm\beta z})}=\frac{G(\underline{k}',i\omega_n\pm\nu)}{(1+e^{\pm\beta(i\omega_n\pm\nu)})}$$

$$=\frac{G(\underline{k}',i\omega_n\pm\nu)}{1+e^{\beta\nu\pm i\beta\omega_n}}=\frac{G(\underline{k}',i\omega_n\pm\nu)}{1-e^{\beta\nu}}$$

Thus, using $G(\underline{k}',\omega'+i\delta)-G(\underline{k}',\omega'-i\delta)=2i\,\mathrm{Im}\,G(\underline{k}',\omega')$ and the fact that the contribution on the circle at infinity vanishes, the self energy becomes

$$\Sigma(\underline{k},i\omega_n)=-\frac{1}{\pi}\sum_{\underline{k}'}\int_{-\infty}^{\infty}\sigma_z\,\mathrm{Im}\,G(\underline{k}',\omega')\sigma_z\Big[\sum_{\alpha}|\bar{g}_{\underline{k}\underline{k}'\alpha}|^2\int_0^{\infty}A_\alpha(\underline{k}-\underline{k}',\nu)$$

$$\left\{\frac{1}{(i\omega_n-\omega'-\nu)(1+e^{-\beta\omega'})}+\frac{1}{(i\omega_n-\omega'+\nu)(1+e^{\beta\omega'})}\right\}d\nu+\frac{V(\underline{k}\underline{k}')}{2}\tanh\frac{\beta\omega'}{2}\Big]d\omega'-$$

$$\sum_{\underline{k}'}\int_0^{\infty}\frac{\sigma_z\{G(\underline{k}',i\omega_n+\nu)+G(\underline{k}',i\omega_n-\nu)\}\sigma_z|\bar{g}_{\underline{k}\underline{k}'\alpha}|^2A(\underline{k}-\underline{k}',\nu)d\nu}{1-e^{\beta\nu}} \qquad 12$$

Letting $i\omega_n\longrightarrow\omega+i\delta$, the self energy can be expressed in terms of the real analytic variable ω (see Schrieffer[5], P. 197). Its most general form is

$$\Sigma(\underline{k},\omega)=\{1-Z(\underline{k},\omega)\}\omega I+\phi(\underline{k},\omega)\sigma_x+\chi(\underline{k},\omega)\sigma_z+\phi^{+}(\underline{k},\omega)\sigma_y. \qquad 13$$

Since the Hamiltonian is invariant with respect to rotations about σ_z in $\underline{\sigma}$ space (σ_x and σ_y are not contained in H), then it is possible to choose phases such that $\phi^{+}(\underline{k},\omega)=0$. Utilizing Eq. 6, Eq. 7, and Eq. 8 one finds the most general expression for the Green function is

$$G(\underline{k},\omega)=\frac{\omega Z(\underline{k},\omega)I+\{\epsilon_{\underline{k}}+\chi(\underline{k},\omega)\}\sigma_z+\phi(\underline{k},\omega)\sigma_x}{\omega^2 Z^2(\underline{k},\omega)-\{\epsilon_{\underline{k}}+\chi(\underline{k},\omega)\}^2+\phi^2(\underline{k},\omega)} \quad . \qquad 14$$

This expression must then be substituted into the free energy yielding a set of four coupled integral equations.

Several steps can be taken to simplify these equations. First, set the quantity $\epsilon'(\underline{k},\omega)=\epsilon_{\underline{k}}+\chi(\underline{k},\omega)$ and let $\Delta(\underline{k},\omega)\equiv\phi(\underline{k},\omega)/Z(\underline{k},\omega)$. Then the following criteria can be used to reduce the algebra considerably:

(1) $\chi(\underline{k},\omega)$, being due to normal coulomb processes, is slowly varying for changes in ω of the Debye frequency and, hence, independent of ω .

(2) $Z(\underline{k},\omega)$ and $\phi(\underline{k},\omega)$ are important mainly at the Fermi level. Since they vary quite slowly with $\underline{k}$, one can set $|\underline{k}|=k_F$.

(3) Since transition metal superconductors are usually impure, it will suffice to determine the spherically averaged self energy because impurity scattering reduces the effects of isotropy.

(4) The chief contribution to the sum over $\underline{k}'$ is when $\epsilon'_{\underline{k}'}\cong\hbar\,\omega_D$. Following essentially the technique of (SSW) the sum over $\underline{k}'$ can be replaced by continuous integration with the following definitions

$$\sum_{\underline{k}'} \rightarrow \int \frac{d^3 k'}{(2\pi)^3} \cong \frac{m\, k_f}{(2\pi)^3} \int d\epsilon_{\underline{k}'}\, d\,\Omega_{\underline{k}'} \qquad 15$$

where $m\, d\epsilon'_{\underline{k}} = k'\, dk'$. Since the chief contribution to the sum over $\underline{k}'$ is near $\epsilon'_{\underline{k}} = \hbar\,\omega_D$, the limits on the integral over $\epsilon'_{\underline{k}}$ can be approximated at $\pm\infty$ respectively and, hence, by residues

$$\int_{-\infty}^{\infty} d\epsilon'_{\underline{k}}\, \sigma_Z\, G(\underline{k}', \omega)\, \sigma_Z = \frac{-i\pi\left[\omega' Z(\omega') I - \phi(\omega')\sigma_X\right]}{\sqrt{\omega'^2 Z^2(\omega') - \phi^2(\omega')}} \qquad 16$$

with the one pole being above the real axis. By averaging Eq. 12 over the spherical part of $\underline{k}$ (and remembering that $i\omega_n \longrightarrow \omega + i\delta$), Eq. 15 and Eq. 16 can be applied to yield for the phonon part of the self energy at $k = k_f$

$$\sum_{PH}(k_f, \omega) = \frac{m\, k_f}{\int d^2k\,(2\pi)^3} \int_0^{\infty} d\omega'\, \mathrm{Re}\left\{\frac{\omega' Z(\omega') I - \phi(\omega')\sigma_X}{\sqrt{\omega'^2 Z^2(\omega') - \phi^2(\omega')}}\right\} \int d^2k \int d\Omega_{\underline{k}'}\, X$$

$$\int_0^{\infty} d\nu \left[A_\alpha(\underline{k}-\underline{k}', \nu)\,|\bar{\sigma}_{\underline{k}\underline{k}'\alpha}|^2 \left\{\frac{1}{(\omega-\omega'-\nu+i\delta)(1+e^{-\beta\omega'})} + \frac{1}{(\omega-\omega'+\nu+i\delta)(1+e^{\beta\omega'})}\right\}\right]$$

$$+ \frac{i m\pi\, k_f}{(2\pi)^3 \int d^2k} \sum_{s=0}^{1} \left\{\frac{\omega_s Z(\omega_s) I - \phi(\omega_s)\sigma_X}{\sqrt{\omega_s^2 Z^2(\omega_s) - \phi^2(\omega_s)}}\right\} \int d^2k \int d\Omega_{\underline{k}'} \int_0^{\infty} d\nu \left[\sum_\alpha \frac{A_\alpha(\underline{k}-\underline{k}', \nu)\,|\bar{\sigma}_{\underline{k}\underline{k}'\alpha}|^2}{1 - e^{\beta\nu}}\right] \qquad 17$$

where $\omega_s = \omega + (-1)^s \nu + i\delta$. Equation 17 can be simplified with the transformation of the negative part of the integral over to the positive portion. Then

$$\Sigma_{PH}(k_f,\omega) = \int_0^\infty Re\left\{\frac{\omega' Z(\omega') I - \phi(\omega')\sigma_x}{\sqrt{\omega'^2 Z^2(\omega') - \phi^2(\omega')}}\right\}\left\{K_\pm(\omega,\omega') f(-\omega') \mp K_\pm(\omega,-\omega') f(\omega')\right\}$$

$$-\frac{i\pi}{(2\pi)^3 \int d^2k} \sum_{s=0}^{1} \left\{\frac{\omega_s Z(\omega_s) I - \phi(\omega_s)\sigma_x}{\sqrt{\omega_s^2 Z^2(\omega_s) - \phi^2(\omega_s)}}\right\} \int d^2k \int \frac{d^2k'}{V_f'} \int_0^\infty d\nu \left[\frac{\sum_\alpha A_\alpha(k-k',\nu)|\bar{g}_{kk'\alpha}|^2}{e^{\beta\nu}-1}\right] \qquad 18$$

where the upper signs belong to factors multiplying the σ_x component only, lower signs belong to factors multiplying the I component only, and

$$K_\pm(\omega,\omega') = \frac{1}{\int d^2k}\int\frac{d^2k'}{V_f}\int d^2k \int_0^\infty d\nu \left[\sum_\alpha |\bar{g}_{kk'\alpha}|^2 A(k-k',\nu)\left\{\frac{1}{\omega+\omega+\nu+i\delta} \pm \frac{1}{\omega'-\omega+\nu-i\delta}\right\}\right]. \qquad 19$$

where the Fermi-Dirac distribution function $f(\omega)$

The coulomb self energy is

$$\Sigma_c(\underline{k}) = -\int\frac{d^3k'}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, Im\left[\sigma_z G(\underline{k}',\omega')\sigma_z\right] V(\underline{k},\underline{k}') \tanh\frac{\beta\omega'}{2}. \qquad 20$$

An approximation is developed for the σ_x component of Σ_c in (SSW) and, hence, only the necessary results will be stated here.

These are

$$\phi_c(k) \cong \phi_c(k_F) = -N(0)\int_0^{10\omega_D} d\omega' \, \mathrm{Re}\left\{\frac{\phi(\omega')U_c}{\sqrt{Z^2(\omega')\omega'^2-\phi^2(\omega')}}\right\}\tanh\frac{\beta\omega'}{2} \qquad 21$$

where the "potential" U_c is approximately

$$U_c = \frac{V_c}{1 + N(0)V_c \ln\left(\epsilon_F/10\,\omega_D\right)} \qquad 22$$

and V_c is the average of the coulomb interaction over the Fermi surface. This finally completes the development of the finite temperature gap equations. It is apparent that, even in reduced form, they are intractable and, thus, some further approximation is needed to bring forth a reasonably accurate set of solutions.

In practice, the gap equations can be solved by computer for the zero temperature case. Finite temperature properties can often then be accurately found from the zero temperature solutions by rules obtained with experimental evidence. From Eq. 18 and Eq. 20, the zero temperature gap equations become

$$\Delta(\omega) = \frac{1}{Z(\omega)}\int_0^{\infty} d\omega' \, \mathrm{Re}\left\{\frac{\Delta(\omega')}{\sqrt{\omega'^2-\Delta^2(\omega')}}\right\}K_+(\omega',\omega)$$

$$-\frac{N(0)}{Z(\omega)}\int_0^{10\omega_D} U_c \, \mathrm{Re}\left\{\frac{\Delta(\omega')}{\sqrt{\omega'^2-\Delta^2(\omega')}}\right\}d\omega' \qquad 23$$

and

$$\left[1-Z(\omega)\right]\omega=\int_0^\infty d\omega'\,\mathrm{Re}\left\{\frac{\omega'}{\sqrt{\omega'^2-\Delta^2(\omega')}}\right\}K_-(\omega',\omega) \qquad 24$$

where $\Delta(\omega)=\phi(\omega)/Z(\omega)$ and $N(0)$ is the electronic density of states at the Fermi level.

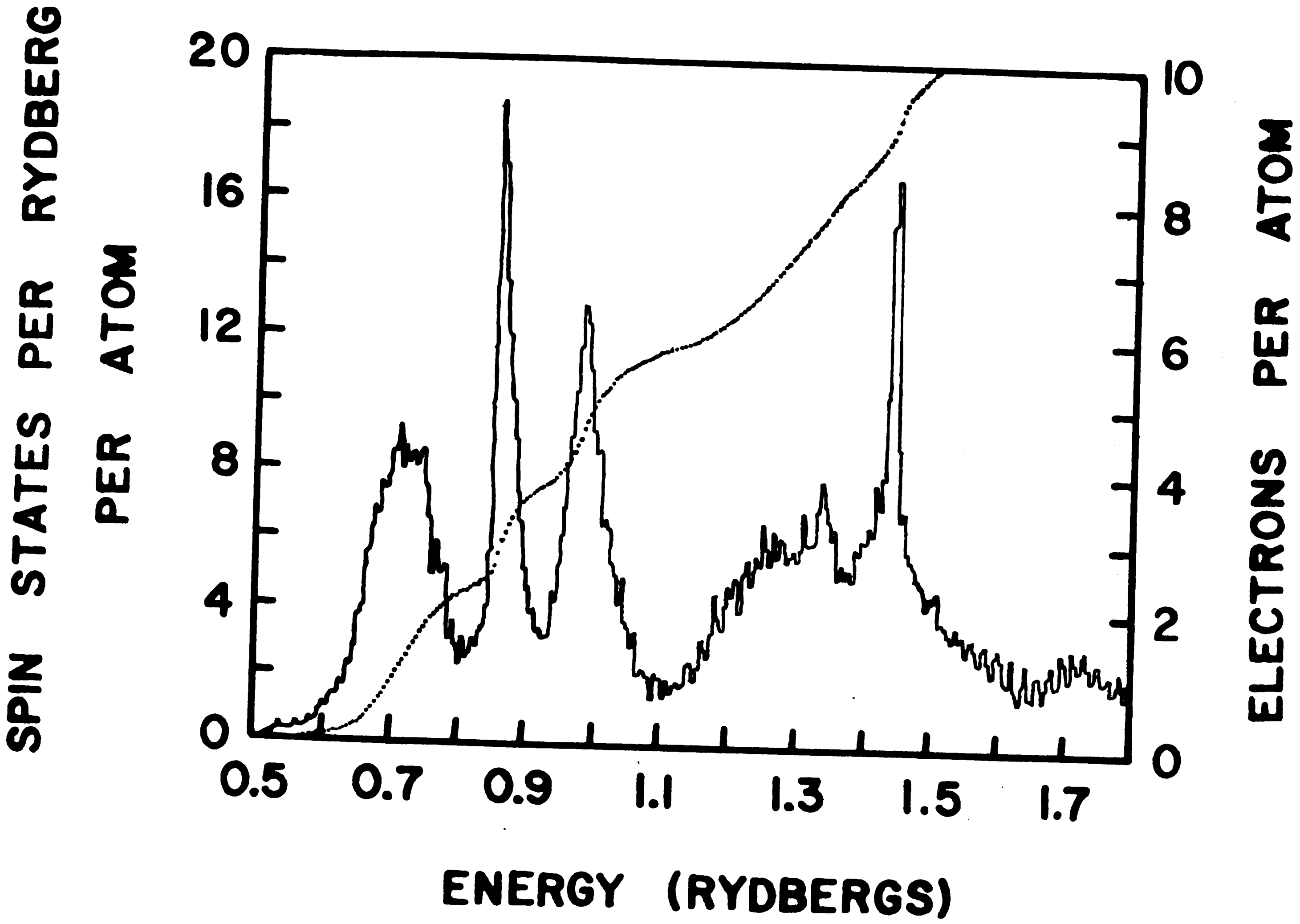

Figure 5. Theoretical density of states for tungsten from band-structure data.

CHAPTER IV

THE ELECTRON-PHONON COUPLING CONSTANT

Derivation of the finite temperature Eliashberg equations begins with the irreducible self energy

$$\Sigma(\underline{k},i\omega_n)=\frac{-1}{\beta}\sum_{\underline{k}',n'}\sigma_{\underline{3}}G(\underline{k}',i\omega_{n'})\sigma_{\underline{3}}\left\{\sum_{\alpha}\left|\bar{g}_{\underline{k},\underline{k}',\alpha}\right|^2 D_{\alpha}\left((\underline{k}-\underline{k}'),i(\omega_n-\omega_{n'})\right)+V(\underline{k}-\underline{k}')\right\}$$

where G and D are the electron and phonon Nambu[30] Green functions respectively, V is the screened coulomb repulsion, and $\bar{g}_{\underline{k},\underline{k}'\alpha}$ is the screened electron-phonon coupling constant. The most important and also most elusive quantity to determine theoretically is $\bar{g}_{\underline{k},\underline{k}'\alpha}$. This constant will be derived as rigorously as possible utilizing Bardeen's self consistent calculation including exchange[32] and other necessary modifications needed to tackle the previously discussed model of groups V and VI transition elements.

Consider the displacement operator of an ion at point due to a lattice wave of wave vector $\underline{q}$ and polarization index α .

$$\delta\underline{R}_m=\frac{\underline{\epsilon}_{\underline{q}\alpha}}{2\sqrt{N}}\left(Q_{\underline{q}\alpha}e^{i\underline{q}\cdot\underline{R}_m}+Q^{+}_{\underline{q}\alpha}e^{-i\underline{q}\cdot\underline{R}_m}\right) \qquad 1$$

where $\underline{\epsilon}_{\underline{q}\alpha}$ is the polarization unit vector for wavevector $\underline{q}$ and polarization index $\alpha = 1, 2, 3$. The normal coordinates are given as

$$Q_{\underline{q}\alpha} = \sqrt{\frac{\hbar}{2M\omega_{\underline{q}\alpha}}}\left(a_{\underline{q}\alpha} + a^{+}_{-\underline{q}\alpha}\right) \qquad 2$$

where $a^{+}_{\underline{q}\alpha}$ and $a_{\underline{q}\alpha}$ are the creation and annihilation operators for phonons of wave vector $\underline{q}$ and polarization index α . Thus the lattice displacement operator at lattice point becomes

$$\delta\underline{R}_m = \frac{1}{2}\sqrt{\frac{\hbar}{2NM\omega_{\underline{q}\alpha}}}\,\epsilon_{\underline{q}\alpha}\, e^{i\underline{q}\cdot\underline{R}_m}\left(a_{\underline{q}\alpha} + a^{+}_{-\underline{q}\alpha}\right) + hc \qquad 3$$

Now assuming that $V(\underline{r})$ is the external potential at distance $\underline{r}$ from the center of a single ion, the potential at point $\underline{R}$ due to displacement of the ion by the amount $\delta\underline{R}$ will be approximated as $V(\underline{r} - \delta\underline{R})$. Then the change in lattice potential at point $\underline{r}$ for a wave of wave vector $\underline{q}$ and polarization index α is

$$V_{\underline{q}\alpha} = \sum_{m}\left[\delta\underline{R}_m \cdot \left\{-\nabla V(\underline{r} - R_m)\right\}\right] \qquad 4$$

where m is summed over the entire lattice. Substituting Eq. 3 into Eq. 4 gives

$$V_{\underline{q}\alpha} = -\frac{1}{2}\sum_{m}\sqrt{\frac{\hbar}{2NM\omega_{\underline{q}\alpha}}}\, e^{i\underline{q}\cdot\underline{R}_m}\left(a_{\underline{q}\alpha}+a^{\dagger}_{-\underline{q}\alpha}\right)\underline{\epsilon}_{\underline{q}\alpha}\cdot\nabla V(\underline{r}-\underline{R}_m) + hC. \qquad 5$$

This is the so-called rigid ion model of Nordheim[33]. Let

$$V(\underline{r}-\underline{R}_m) = \sum_{\underline{L}} V_{\underline{L}}\, e^{i\underline{L}\cdot(\underline{r}-\underline{R}_m)} . \qquad 6$$

Then,

$$V_{\underline{q}\alpha} = -\frac{1}{2}\sqrt{\frac{\hbar}{2NM\omega_{\underline{q}\alpha}}}\left(a_{\underline{q}\alpha}+a^{\dagger}_{-\underline{q}\alpha}\right)\sum_{\underline{L},m} V_{\underline{L}}\left(i\underline{L}\cdot\underline{\epsilon}_{\underline{q}\alpha}\right)e^{i\underline{L}\cdot\underline{r}}\,e^{i(\underline{q}-\underline{L})\cdot\underline{R}_m} + hC. \qquad 7$$

Since

$$\sum_{m} e^{i(\underline{q}-\underline{L})\cdot\underline{R}_m} = \sum_{n} N\,\delta_{\underline{L},\,\underline{q}+\underline{G}_n} \qquad 8$$

where $\underline{G}_n$ is the nth reciprocal lattice vector. Then

$$V_{\underline{q}\alpha} = -\frac{i}{2}\sqrt{\frac{N\hbar}{2M\omega_{\underline{q}\alpha}}}\left(a_{\underline{q}\alpha}+a^{\dagger}_{-\underline{q}\alpha}\right)\sum_{n} V_{\underline{q}+\underline{G}_n}\left(\underline{q}+\underline{G}_n\right)\underline{\epsilon}_{\underline{q}\alpha}\, e^{i(\underline{q}+\underline{G}_n)\cdot\underline{r}} + hC. \qquad 9$$

The total electron-phonon interaction Hamiltonian for scattering of an electron from state $\underline{k},s$ to state $\underline{k}',s$ is just the matrix element of $V_{\underline{q}\alpha}$ between states $\underline{k},s$ and $\underline{k}',s$ multiplied by $C^{\dagger}_{\underline{k}',s}C_{\underline{k},s}$ which destroys an electron in state $\underline{k},s$ and recreates it in $\underline{k}',s$. So one can then write

I

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$$H_{e-Ph} = \sum_{\underline{k},\underline{k}',s,\alpha} g_{\underline{k},\underline{k}'\alpha}\, C^{+}_{\underline{k}'s} C_{\underline{k}s} \left(a_{\underline{q}\alpha} + a^{+}_{-\underline{q}\alpha}\right) \qquad 10$$

letting

$$\underline{k} - \underline{k}' = \underline{q} + \underline{G}_n$$

and where

$$g_{\underline{k}\underline{k}'\alpha} = -\frac{i}{2}\sqrt{\frac{N\hbar}{2M\omega_{\underline{k}\underline{k}'\alpha}}}\,(\underline{k}-\underline{k}')\cdot\epsilon_{\underline{k}\underline{k}'\alpha} V_{\underline{k}-\underline{k}'} \langle \underline{k}|\, e^{i(\underline{k}-\underline{k}')\cdot\underline{r}}\, |\underline{k}'\rangle + hc \qquad 11$$

Subscripts $\underline{q}$ may be replaced by $\underline{k}\ \underline{k}'$ since q is unique for a given $\underline{k}\ \underline{k}'$ and the sum over reciprocal lattice vectors is inferred in the sum over $\underline{k}\ \underline{k}'$ because G_n is also unique for a given $\underline{k}\ \underline{k}'$ in umklapp processes[34]. The best way to determine $g_{\underline{k}\underline{k}'\alpha}$ is to find

$$M(\underline{k},\underline{k}')_\alpha = \langle n_{\underline{q}\alpha}|\langle 0_{\underline{k}'s}|H_{e-PH}|1_{\underline{k}s}\rangle|n_{\underline{q}\alpha}-1\rangle \qquad 12$$

which gives

$$M(\underline{k},\underline{k}')_\alpha = \bar{g}_{\underline{k},\underline{k}'\alpha}\sqrt{n_{\underline{q}\alpha}}\,. \qquad 13$$

[37]

To begin the Bardeen calculation it is necessary to return to

$$V_{\underline{q}\alpha}=-\frac{1}{2}\sqrt{\frac{\hbar}{2NM\omega_{\underline{q}\alpha}}}\left(a_{\underline{q}\alpha}+a^{+}_{-\underline{q}\alpha}\right)\sum_{m}e^{i\underline{q}\cdot\underline{R}_m}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\nabla V(\underline{r}-\underline{R}_m)+hc \qquad 5$$

or

$$V_{\underline{q}\alpha}=\frac{-\sqrt{n_{\underline{q}\alpha}}}{2}\sqrt{\frac{\hbar}{2NM\omega_{\underline{q}\alpha}}}\sum_{m}e^{i\underline{q}\cdot\underline{R}_m}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\nabla V(\underline{r}-\underline{R}_m)+hc \qquad 14$$

whose phonon number eigenvalue has been determined in phonon occupation number space. Let $V_{\underline{q}\alpha}$ operate upon a conduction electron state $|\underline{k}\rangle$ as

$$V_{\underline{q}\alpha}|\underline{k}\rangle=\sum_{n}\left\{V^{(nc)}_{+\underline{q}\alpha}|\underline{k}+\underline{q}+\underline{G}_n\rangle+V^{(nc)}_{-\underline{q}\alpha}|\underline{k}-\underline{q}-\underline{G}_n\rangle\right\} \qquad 15$$

where

$$V^{(nc)}_{+\underline{q}\alpha}=\langle\underline{k}+\underline{q}+\underline{G}_n|V_{\underline{q}\alpha}|\underline{k}\rangle \qquad 16a$$

and

$$V^{(nc)}_{-\underline{q}\alpha}=\langle\underline{k}-\underline{q}-\underline{G}_n|V_{\underline{q}\alpha}|\underline{k}\rangle. \qquad 16b$$

Doing the same to a d-electron state $|\underline{K}\rangle$

$$V_{\underline{q}\alpha}|\underline{K}\rangle=\sum_{n}\left\{V^{(nd)}_{+\underline{q}\alpha}|\underline{K}+\underline{q}+\underline{G}_n\rangle+V^{(nd)}_{\underline{q}\alpha}|\underline{K}-\underline{q}-\underline{G}_n\rangle\right\} \qquad 17$$

where

$$V_{+\underline{q}\alpha}^{(nd)} = \langle \underline{K}+\underline{q}+\underline{G}_n | V_{\underline{q}\alpha} | \underline{K} \rangle \qquad 18a$$

$$V_{-\underline{q}\alpha}^{(nd)} = \langle \underline{K}-\underline{q}-\underline{G}_n | V_{\underline{q}\alpha} | \underline{K} \rangle . \qquad 18b$$

This represents the action upon a core electron by a lattice wave of wave vector $\underline{q}$ and polarization α. To be self-consistent, one must also determine how the electron states are perturbed by such a lattice wave.

For the screening effect, expand the perturbed electronic states $|\underline{k}\rangle\rangle$ and $|\underline{K}\rangle\rangle$ in terms of

$$|\underline{k}\rangle\rangle = |\underline{k}\rangle + \sum_{n} \left\{ a_{\underline{q}\alpha}(\underline{k}n) |\underline{k}+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}n) |\underline{k}-\underline{q}-\underline{G}_n\rangle \right\} \qquad 19a$$

and

$$|\underline{K}\rangle\rangle = |\underline{K}\rangle + \sum_{n} \left\{ A_{\underline{q}\alpha}(\underline{K}n) |\underline{K}+\underline{q}+\underline{G}_n\rangle + B_{\underline{q}\alpha}(\underline{K}n) |\underline{K}-\underline{q}-\underline{G}_n\rangle \right\} \qquad 19b$$

to first order where a, b, A and B are small perturbation coefficients. These latter two equations, when summed over all of the states of the band in question, are the net response of that particular band to first order due to the motion of the ions plus the screening effect of the other band. Next, call the Hartree-Fock potential energy of the d plus conduction-electrons V_ρ^0. Operating with V_ρ^0 upon a perturbed state using

$$V_\rho^0|\underline{k}\rangle\rangle = e^2\sum(\underline{k}')\{\langle\underline{k}'|1/R|\underline{k}'\rangle|\underline{k}\rangle\rangle - \langle\underline{k}'|1/R|\underline{k}\rangle\rangle|\underline{k}'\rangle\}$$
$$+ e^2\sum(K')\{\langle\underline{K}'|1/R|\underline{K}'\rangle|\underline{k}\rangle\rangle - \langle\underline{K}'|1/R|\underline{k}\rangle\rangle|\underline{K}'\rangle\} \qquad \text{20a}$$

$$V_\rho^0|\underline{K}\rangle\rangle = e^2\sum(\underline{K}')\{\langle\underline{K}'|1/R|\underline{K}'\rangle|\underline{K}\rangle\rangle - \langle\underline{K}'|1/R|\underline{K}\rangle\rangle|\underline{K}'\rangle$$
$$+ e^2\sum(\underline{k}')\{\langle\underline{k}'|1/R|\underline{k}'\rangle|\underline{K}\rangle\rangle - \langle\underline{k}'|1/R|\underline{K}\rangle\rangle|\underline{k}'\rangle\} \qquad \text{20b}$$

with the specification that the eigenvectors span spin space as well as Hilbert space and that the sums include spin. Call the Hartree-Fock potential energy in the perturbed lattice V_ρ^T . Then

$$V_\rho^T|\underline{k}\rangle\rangle = e^2\sum(\underline{k}')\{\langle\langle\underline{k}'|1/R|\underline{k}'\rangle\rangle|\underline{k}\rangle\rangle - \langle\langle\underline{k}'|1/R|\underline{k}\rangle\rangle|\underline{k}'\rangle\rangle\}$$
$$+ e^2\sum(\underline{K}')\{\langle\langle\underline{K}'|1/R|\underline{K}'\rangle\rangle|\underline{k}\rangle\rangle - \langle\langle\underline{K}'|1/R|\underline{k}\rangle\rangle|\underline{K}'\rangle\rangle\} \qquad \text{21a}$$

$$V_\rho^T|\underline{K}\rangle\rangle = e^2\sum(\underline{K}')\{\langle\langle\underline{K}'|1/R|\underline{K}'\rangle\rangle|\underline{K}\rangle\rangle - \langle\langle\underline{K}'|1/R|\underline{K}\rangle\rangle|\underline{K}'\rangle\rangle\}$$
$$+ e^2\sum(\underline{k}')\{\langle\langle\underline{k}'|1/R|\underline{k}'\rangle\rangle|\underline{K}\rangle\rangle - \langle\langle\underline{k}'|1/R|\underline{K}\rangle\rangle|\underline{k}'\rangle\rangle\} \qquad \text{21b}$$

is the effect upon a particular bandstate perturbed by the bare ion and screened by the other non-core electrons. Now substitute Eq. 19 into Eq. 21 and subtract Eq. 20 to get

$$
\begin{aligned}
&V_\rho|\underline{k}\rangle\rangle=(V_\rho^T-V_\rho^0)|\underline{k}\rangle\rangle\\
&=e^2\sum_n(\underline{k}')\Big[\{a^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}'\rangle+a_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_n\rangle\\
&\quad+b^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}'\rangle+b_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_n\rangle\}|\underline{k}\rangle\rangle\\
&\quad-\{a^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\rangle+a_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_n\rangle\rangle\\
&\quad+b^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\rangle+b_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_n\rangle\rangle\}\Big]\\
&\quad+e^2\sum_n(\underline{K}')\Big[\{A^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{K}'\rangle+A_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{K}'+\underline{q}+\underline{G}_n\rangle\\
&\quad+B^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{K}'\rangle+B_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{K}'-\underline{q}-\underline{G}_n\rangle\}|\underline{k}\rangle\rangle\\
&\quad-\{A^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}\rangle|\underline{K}'\rangle\rangle+A_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{k}\rangle|\underline{K}'+\underline{q}+\underline{G}_n\rangle\rangle\\
&\quad+B^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}\rangle|\underline{K}'\rangle\rangle+B_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{k}\rangle|\underline{K}'-\underline{q}-\underline{G}_n\rangle\rangle\}\Big] \qquad 22
\end{aligned}
$$

and an identical expression with K and k, a and A, and b and B interchanged.

Equation 22 represents the change in potential energy of an electron within a given band interacting with a bare lattice wave of wavevector $\underline{q}$ and polarization α when properly screened by all of the other electrons in both bands.

It is now necessary to solve the Schrodinger equation for the perturbation expansion coefficients. For the unperturbed lattice, Schrodinger's equation is

$$H_0|\underline{k}\rangle + V_0|\underline{k}\rangle = E_0(\underline{k})|\underline{k}\rangle \qquad \text{23a}$$

for the conduction electrons and

$$H_0|\underline{K}\rangle + V_0|\underline{K}\rangle = E_0(\underline{K})|\underline{K}\rangle \qquad \text{23b}$$

for the d-band electrons where V_0 includes all of the potential fields acting upon an electron within a particular band in an undistorted crystal. Now, for a lattice perturbed by a wave of wavevector $\underline{q}$ and polarization α, the Schrodinger equation becomes

$$H_0|\underline{k}\rangle\rangle + (V_0 + V_{\underline{q}\alpha} + V_p)|\underline{k}\rangle\rangle = E(\underline{k})|\underline{k}\rangle\rangle \qquad \text{24}$$

for the conduction electrons and

$$H_0|\underline{K}\rangle\rangle + (V_0 + V_{\underline{q}\alpha} + V_p)|\underline{K}\rangle\rangle = E(\underline{K})|\underline{K}\rangle\rangle \qquad \text{25}$$

for d-band electrons. Substitution of the perturbation expansions Eq. 22 into equations Eq. 24 and then subtracting Eq. 23 and including the assumption that $E(k) = E_0(k)$ and $E(K) = E_0(K)$ gives

$$
\begin{aligned}
&\sum\{a_{\underline{q}\alpha}(\underline{k}n)H_0|\underline{k}+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}n)H_0|\underline{k}-\underline{q}-\underline{G}_n\rangle\}\\
&+V_0\sum_n\{a_{\underline{q}\alpha}(\underline{k}n)|\underline{k}+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}n)|\underline{k}-\underline{q}-\underline{G}_n\rangle\}\\
&+\sum_n\{V_{+\underline{q}\alpha}^{(nc)}|\underline{k}+\underline{q}+\underline{G}_n\rangle + V_{-\underline{q}\alpha}^{(nc)}|\underline{k}-\underline{q}-\underline{G}_n\rangle\}\\
&+\sum_n\Big[a_{\underline{q}\alpha}(\underline{k}n)\{V_{+\underline{q}\alpha}^{(nc)}|\underline{k}+2\underline{q}+2\underline{G}_n\rangle + V_{-\underline{q}\alpha}^{(nc)}|\underline{k}\rangle\}\\
&\qquad\qquad + b_{\underline{q}\alpha}^{(nc)}(\underline{k}n)\{V_{+\underline{q}\alpha}^{(nc)}|\underline{k}\rangle + V_{-\underline{q}\alpha}^{(nc)}|\underline{k}-2\underline{q}-2\underline{G}_n\rangle\}\Big]\\
&+e^2\sum_n(\underline{k}')\Big[a^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}'\rangle + b^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}'\rangle\\
&+a_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_n\rangle\Big]|\underline{k}\rangle\\
&-e^2\sum_n(\underline{k}')\Big[\{a^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}\rangle + b^*_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}\rangle\}|\underline{k}'\rangle\\
&+\{a_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}|R^{-1}|\underline{k}'\rangle|\underline{k}'+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}'n)\langle\underline{k}|R^{-1}|\underline{k}'\rangle|\underline{k}'-\underline{q}-\underline{G}_n\rangle\}\Big]\\
&+e^2\sum_n(\underline{K}')\Big[A^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{K}'\rangle + B^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{K}'\rangle\\
&+A_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{K}'+\underline{q}+\underline{G}_n\rangle + B_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'|R^{-1}|\underline{K}'-\underline{q}-\underline{G}_n\rangle\Big]|\underline{k}\rangle\\
&-e^2\sum_n(\underline{K}')\Big[\{A^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'+\underline{q}+\underline{G}_n|R^{-1}|\underline{k}\rangle + B^*_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{K}'-\underline{q}-\underline{G}_n|R^{-1}|\underline{k}\rangle\}|\underline{K}'\rangle\\
&+\{A_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{k}|R^{-1}|\underline{K}'\rangle|\underline{K}'+\underline{q}+\underline{G}_n\rangle + B_{\underline{q}\alpha}(\underline{K}'n)\langle\underline{k}|R^{-1}|\underline{K}'\rangle|\underline{K}'-\underline{q}-\underline{G}_n\rangle\}\Big]\\
&=E(\underline{k})\sum_n\{a_{\underline{q}\alpha}(\underline{k}n)|\underline{k}+\underline{q}+\underline{G}_n\rangle + b_{\underline{q}\alpha}(\underline{k}n)|\underline{k}-\underline{q}-\underline{G}_n\rangle\}
\end{aligned}
\tag{25}
$$

for conduction electrons and an identical expression with K and k, A and a, and B and b interchanged for the d-band electrons. Now operate with bravectors $\langle \underline{k}+\underline{q}+\underline{G}_n|$ and $\langle \underline{k}-\underline{q}-G_n|$ upon Eq. 25a and with bravectors $\langle \underline{K}+\underline{q}+\underline{G}_n|$ and $\langle \underline{K}-\underline{q}-G_n|$ upon Eq. 25b to get four equations containing the expansion coefficients where the remaining terms containing H_0 and V_0 in Eq. 25 are removed by subtracting the Schrodinger equation containing them. These equations are

$$0=V_{+\underline{q}\alpha}^{(nc)}+\{E(\underline{k}+\underline{q}+\underline{G}_n)-E(\underline{k})\}A_{\underline{q}\alpha}(\underline{k}n)$$

$$+e^2\sum_m(\underline{k}')\Big[a^*_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$+\;b^*_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$+\;a_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{k}\rangle$$

$$+\;b_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle\Big]$$

$$-e^2\sum_m(\underline{k}')\Big[a^*_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle$$

$$+\;b^*_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle$$

$$+\;a_{\underline{q}\alpha}(\underline{k}'m)\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle$$

$$+b_{\underline{q}\alpha}(\underline{k}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\Big]$$

$$+e^2\sum_m(\underline{K}')\Big[A^*_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{K}'\rangle|\underline{k}\rangle$$

$$+B^*_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{K}'\rangle|\underline{k}\rangle$$

$$+A_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'|R^{-1}|\underline{K}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle$$

$$+B_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'|R^{-1}|\underline{K}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle\Big]$$

$$+e\sum_m(\underline{K}')\Big[A^*_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{K}'\rangle$$

$$+B^*_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{K}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{K}'\rangle$$

$$+A_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}|R^{-1}|\underline{K}'\rangle|\underline{K}'+\underline{q}+\underline{G}_m\rangle$$

$$+B_{\underline{q}\alpha}(\underline{K}'m)\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}|R^{-1}|\underline{K}'\rangle|\underline{K}'-\underline{q}-\underline{G}_m\rangle\Big] \qquad 27$$

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and, again, a similar expression for conduction electrons. The expressions for $b_{\underline{q}\alpha}$ and $B_{\underline{q}\alpha}$ are identical with Eq. 26 and Eq. 27 respectively except that $+\underline{q}+G_n$ becomes $-\underline{q}-G_n$ and $V_{+\underline{q}\alpha}$ becomes $V_{-\underline{q}\alpha}$. Moreover, they contain no additional information. Equations 26 and 27 may be rearranged to give an explicit expression for the coefficient multiplying the energy difference in these equations. The perturbation coefficients are

$$a_{\underline{q}\alpha}(\underline{k}n)=M(\underline{k},\underline{k}+\underline{q}+G_n)_\alpha/\{E(\underline{k})-E(\underline{k}+\underline{q}+\underline{G}_n)\} \qquad 28$$

$$b_{\underline{q}\alpha}(\underline{k}n)=M(\underline{k},\underline{k}-\underline{q}-G_n)_\alpha/\{E(\underline{k})-E(\underline{k}-\underline{q}-\underline{G}_n)\} \qquad 29$$

$$A_{\underline{q}\alpha}(\underline{K}n)=M(\underline{K},\underline{K}-\underline{q}-G_n)_\alpha/\{E(\underline{K})-E(\underline{K}+\underline{q}+\underline{G}_n)\} \qquad 30$$

$$B_{\underline{q}\alpha}(\underline{K}n)=M(\underline{K},\underline{K}-\underline{q}-G_n)_\alpha/\{E(\underline{K})-E(\underline{K}-\underline{q}-\underline{G}_n)\} \qquad 31$$

Now substitute these expressions for the coefficients into Eq. 26 and Eq. 27 and solve. The result is

$$M(\underline{k},\underline{k}+\underline{q}+\underline{G}_n)_\alpha = V_{+\underline{q}\alpha} + e^2 \sum_m(\underline{k}')$$

$$\Bigg[\frac{M^*(\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\Big)$$

$$+\frac{M^*(\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}\rangle\Big)$$

$$+\frac{M(\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle\Big)$$

$$+\frac{M(\underline{k}',\underline{k}-\underline{q}-\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\Big)\Bigg]$$

$$+e^2\sum_m(\underline{k}')$$

$$\Bigg[\frac{M(\underline{k}',\underline{k}+\underline{q}+\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\Big)$$

$$+\frac{M^*(\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\Big(\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{K}\rangle$$

$$-\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{K}\rangle|\underline{k}'\rangle\Big)$$

$$+\frac{M(\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\Big(\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{K}\rangle$$

$$-\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{K}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle\Big)$$

$$+\frac{M(\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m)_\alpha}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\Big(\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{K}\rangle$$

$$-\langle\underline{K}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{K}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\Big]\qquad 32$$

for d electrons coupled with an identical expression for conduction electrons with k and K, a and A and b and B interchanged. Before writing down an expression for the electron-phonon coupling constant, the equations

$$V_{+\underline{q}\alpha}^{(hc)}=-\frac{1}{2}\sqrt{\frac{\hbar\, n_{q\alpha}}{2NM\,\omega_{\underline{q}\alpha}}}\sum_m e^{i\underline{q}\cdot\underline{R}_m}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\langle\underline{k}+\underline{q}+\underline{G}_n|\nabla V(\underline{r}-\underline{R}_m)|\underline{k}\rangle+hc \qquad 16a$$

$$V_{-\underline{q}\alpha}^{(nc)}=\frac{1}{2}\sqrt{\frac{\hbar\, n_{q\alpha}}{2NM\omega_{\underline{q}\alpha}}}\sum_m e^{i\underline{q}\cdot\underline{R}_m}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\langle\underline{k}-\underline{q}-G_n|\nabla V(\underline{r}-R_m)|\underline{k}\rangle+hc \qquad 16b$$

$$V_{+\underline{q}\alpha}^{(nd)}=\frac{1}{2}\sqrt{\frac{\hbar\, n_{\underline{q}\alpha}}{2NM\omega_{\underline{q}\alpha}}}\sum_m e^{i\underline{q}\cdot\underline{R}_m}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\langle\underline{K}+\underline{q}+\underline{G}_n|\nabla V(\underline{r}-\underline{R}_m)|\underline{K}\rangle+hc \qquad 18a$$

$$V^{-(nd)}_{-\underline{q}\alpha} = -\frac{1}{2}\sqrt{\frac{\hbar\, n_{\underline{q}\alpha}}{2NM\omega_{\underline{q}\alpha}}}\sum_{m} e^{i\underline{q}\cdot\underline{R}_m}\,\epsilon_{\underline{q}\alpha}\cdot\langle\underline{K}-\underline{q}-G_n|\nabla V(\underline{r}-\underline{R}_m)|\underline{K}\rangle + hc. \qquad 18b$$

can be simplified. First, Bloch's theorem states that

$$\psi_{\underline{k}}(\underline{r}+\underline{R}_m) = e^{i\underline{k}\cdot\underline{R}_m}\psi_{\underline{k}}(\underline{r}).$$

Thus

$$\langle\underline{k}|\nabla V(\underline{r}-\underline{R}_m)|\underline{k}'\rangle = \int\psi^*_{\underline{k}}(\underline{r})\nabla V(\underline{r}-\underline{R}_m)\psi_{\underline{k}'}(\underline{r})d\underline{r}$$

$$= \int\psi^*_{\underline{k}}(\underline{r}-\underline{R}_m)e^{-i\underline{k}\cdot\underline{R}_m}\nabla V(\underline{r}-\underline{R}_m)\psi_{\underline{k}'}(\underline{r}-\underline{R}_m)e^{i\underline{k}'\cdot\underline{R}_m}d(\underline{r}-\underline{R}_m)$$

$$= e^{i(\underline{k}'-\underline{k})\cdot\underline{R}_m}\int\psi^*_{\underline{k}}(\underline{r}-\underline{R}_m)\nabla V(\underline{r}-\underline{R}_m)\psi_{\underline{k}'}(\underline{r}-\underline{R}_m)d(\underline{r}-\underline{R}_m)$$

$$= e^{i(\underline{k}'-\underline{k})\cdot\underline{R}_m}\int\psi^*_{\underline{k}}(\underline{r})\nabla V(\underline{r})\psi_{\underline{k}}(\underline{r})\,d(\underline{r})$$

$$= e^{i(\underline{k}'-\underline{k})\cdot\underline{R}_m}\langle\underline{k}|\nabla V(\underline{r})|\underline{k}'\rangle \qquad 33$$

Next, multiply by $e^{i\underline{q}\cdot\underline{R}_m}$ and sum over all lattice sites

$$\sum_m e^{i\underline{q}\cdot\underline{R}_m} e^{i(\underline{k}'-\underline{k})\cdot\underline{R}_m}\langle\underline{k}|\nabla V(\underline{r})|\underline{k}'\rangle=\langle\underline{k}|\nabla V(\underline{r})|\underline{k}+\underline{q}+\underline{G}_n\rangle N \qquad 34$$

Equation 34 can now be used in Eq. 16 and Eq. 18 and these equations in turn are substituted into Eq. 32 and Eq. 33. Using Eq. 13, the expression for the electron-phonon coupling constant is

$$\bar{g}_{\underline{k},\underline{k}+\underline{q}+\underline{G}_n,\alpha}=-\sqrt{\frac{\hbar N}{2M\omega_{\underline{q}\alpha}}}\,\epsilon_{\underline{q}\alpha}\cdot\langle\underline{k}|\nabla V(\underline{r})|\underline{k}+\underline{q}+\underline{G}_n\rangle$$

$$e^2\sum_m(\underline{k}')\times$$

$$\Big[\Big\{\Big(\frac{\bar{g}^*_{\underline{k}',\underline{k}+\underline{q}+\underline{G}_m\alpha}}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\Big)\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\Big)\Big\}$$

$$+\Big\{\Big(\frac{\bar{g}_{\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}+\underline{q}+\underline{G}_m)}\Big)\Big(\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{k}\rangle$$

$$-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle\Big)\Big\}$$

$$+\left\{\left(\frac{\bar{\delta}^{*}_{\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right)\left(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle\right.\right.$$

$$\left.\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\right)\right\}$$

$$+\left\{\left(\frac{\bar{\delta}_{\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right)\left(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle\right.\right.$$

$$\left.\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\right)\right\}\Big]$$

$$+e^2\sum_{m}(\underline{k}')\times$$

$$\Big[\left\{\left(\frac{\bar{\delta}^{*}_{\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\right)\left(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle\right.\right.$$

$$\left.\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\right)\right\}$$

$$+\left\{\left(\frac{\bar{\delta}_{\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\right)\left(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{k}\rangle\right.\right.$$

$$\left.\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle\right)\right\}$$

$$+\left\{\left(\frac{\bar{\delta}^{*}_{\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right)\Big(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle\right.$$

$$\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\Big)\right\}$$

$$+\left\{\left(\frac{\bar{\delta}_{\underline{k}',\underline{k}'-\underline{q}-\underline{G}_m,\alpha}}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right)\Big(\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle\right.$$

$$\left.-\langle \underline{k}+\underline{q}+\underline{G}_n|\langle \underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\Big)\right\}\Bigg] \qquad 35$$

for conduction electrons coupled with a similar expression for the d-band electrons. Only the first term in Eq. 35 represents the unscreened electron-phonon coupling constant whereas the remaining terms under the sum are entirely due to screening.

The problem now is to determine the bare ion potential $V(\underline{r})$. This potential may be broken down into two parts, one of which is the nuclear coulomb potential and the other being due to the screening effect (including exchange) of the core electrons. Since the core electrons all lie within closed shells, their potential is spherically symmetric about the nucleus and hence the vector notation $(\underline{r})$ may be dropped. Since five or six atomic electrons enter band states in the transition metals in question, then the remaining core will be quite small and should resemble their atomic counterparts quite closely. In fact the use of atomic potentials to represent core potentials may very well be a better approximation for transition metals than for normal metals. The calculation of these potentials is largely unnecessary due to the efforts of Herman and Skillman[26]. Essentially, they have determined a set of self-consistent Hartree-Fock potentials for neutral atomic elements. It is from these numerical potentials and radial densities that the necessary core potentials must be determined.

Up until now the possibility of phonon induced interband transitions has not been considered. The reason so is that such transition probabilities would be proportional to matrix elements of the type $\langle \underline{K} | \nabla V(r) | \underline{k} + \underline{q} + \underline{G}_n \rangle$ and $\langle \underline{k} | \nabla V(r) | \underline{K} + \underline{q} + \underline{G}_n \rangle$. Since the potential $V(r)$ and hence its gradient is spherically symmetric, these matrix elements can be non zero only if the bra and ket contain at least one identical spherical harmonic. However, in specifying the wavefunctions, such a possibility was eliminated. Thus, for this particular model, interband transitions are ruled out.

CHAPTER V

EVALUATION OF MATRIX ELEMENTS

The purpose of this section is to develop specific expressions for matrix elements of the type

$$\langle P_1(\underline{r}')|\langle P_2(\underline{r})|1/|\underline{r}-\underline{r}'|\,|P_3(\underline{r})\rangle|P_4(\underline{r}')\rangle$$

and

$$\langle P_1(\underline{r})|\nabla V(r)|P_2(\underline{r})\rangle$$

where $\nabla V(r)$ is the gradient of the bare ion potential. The form of the wavefunctions will be linear combinations of atomic orbitals and plane waves from which any orthogonalized plane wave can be formed.

Part A - Fourier Coefficients of Wavefunctions

Consider a linear combination of atomic orbitals

$$\Lambda_{\underline{k}}^{nlm}(\underline{r}) = \frac{1}{\sqrt{N}} \sum_{j} e^{i\underline{k}\cdot\underline{r}_j} \phi_{nlm}(\underline{r}-\underline{r}_j) \qquad 1$$

where N is the total number of lattice points, r_j is the jth lattice point, and ϕ is a given atomic wavefunction having quantum numbers n, l, and m respectively. The Fourier transform is

$$C_{\underline{k}}^{nlm}(\underline{P}) = \frac{1}{(2\pi)^3} \int e^{i\underline{P}\cdot\underline{r}} \Lambda^{nlm}(\underline{r})\, d\underline{r} \qquad 2$$

Performing the integration, this coefficient then becomes

$$C_{\underline{k}}^{nlm}(\underline{P})=\frac{1}{(2\pi)^3 N^{1/2}}\sum_j e^{i(\underline{k}+\underline{P})\cdot\underline{r}_j}\, I^{nlm}_{(P,\theta_P)} \qquad 3$$

or

$$C_{\underline{k}}^{nlm}(P)=\frac{N^{1/2}\,\delta_{\underline{P},-\underline{k}}}{(2\pi)^3}\, I^{nlm}_{(P,\theta_P)} \qquad 4$$

where

$$I^{nlm}_{(P,\theta_P)}=\int e^{i\underline{P}\cdot\underline{r}}\,\phi_{nlm}(\underline{r})\,d\underline{r}\,. \qquad 5$$

Orthogonalized plane waves may now be treated using

$$C_{\underline{k}}^{OPW}(\underline{P})=\frac{1}{(2\pi)^3}\int e^{i\underline{P}\cdot\underline{r}}\,\psi_{\underline{k}}(\underline{r})\,d\underline{r} \qquad 6$$

or

$$C_{\underline{k}}^{OPW}(\underline{P})=\frac{V^{-\frac{1}{2}}}{(2\pi)^3}\int e^{i\underline{P}\cdot\underline{r}}\Big\{e^{i\underline{k}\cdot\underline{r}} -\sum\Big(\int e^{i\underline{k}\cdot(\underline{r}'-\underline{r}_j)}\,\phi_{nlm}(\underline{r}'-\underline{r}_j)\,d\underline{r}'\Big)e^{i\underline{k}\cdot\underline{r}_j}\,\phi_{nlm}(\underline{r}-\underline{r}_j)\Big\}\,d\underline{r}\,. \qquad 7$$

The integrations are then performed to give

$$C_{k}^{OPW}(\underline{P})=\frac{V^{\frac{1}{2}}\,\delta_{\underline{P},-\underline{k}}}{(2\pi)^3}-\frac{N^{\frac{1}{2}}}{V^{\frac{1}{2}}}\sum_{n=1}^{n_{max}}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} I^{nlm}(k,-\theta_k)\, C_{\underline{k}}^{nlm}(P)\,. \qquad 8$$

Likewise, proper linear combinations of d-states having T_{2g} symmetry possess the coefficients

$$C_{\underline{k}}^{xy}(\underline{P}) = \frac{C_{\underline{k}}^{n22} - C_{\underline{k}}^{n2-2}}{\sqrt{2}}, \qquad 9a$$

$$C_{\underline{k}}^{yz}(\underline{P}) = \frac{C_{\underline{k}}^{n21} + C_{\underline{k}}^{n2-1}}{\sqrt{2}}, \qquad 9b$$

and

$$C_{\underline{k}}^{zx}(\underline{P}) = \frac{-C_{\underline{k}}^{n21} + C_{\underline{k}}^{n2-1}}{\sqrt{2}}. \qquad 9c$$

To evaluate I^{nlm}, let

$$\phi_{nlm}(\underline{r}) = R_{nl}(r)\, Y_l^m(\theta,\phi) \qquad 10$$

and

$$e^{i\underline{P}\cdot\underline{r}} = \sqrt{4\pi}\sum_{l'=0}^{\infty}(2l'+1)^{1/2}\, j_{l'}(Pr)\, Y_{l'}^{0}(\theta'). \qquad 11$$

Transform from the primed to unprimed coordinate system letting θ_p be the angle between Z' and Z. Then (see Edmonds[38]),

$$Y_{l'}^{0}(\theta') = \sum_{m'=-l}^{l} Y_{l'}^{m'}(\theta,\phi)\sqrt{\frac{(l'-m')!}{(l'+m')!}}\, P_{l'}^{m'}(\cos\theta_p). \qquad 12$$

Thus

$$I^{nlm}(P,\theta_p)=\sqrt{4\pi}\sum_{l'=0}^{\infty}(2l'+1)^{1/2}\sum_{m'=-l}^{l}\sqrt{\frac{(l'-m')!}{(l'+m')!}}\,P_{l'}^{m'}(\cos\theta_p) \qquad 13$$

$$\times\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi}R_{nl}(r)\,j_{l'}(Pr)\,Y_{l'}^{m'}(\theta,\phi)\,Y_{l}^{m}(\theta,\phi)\,r^2\sin\theta\,d\theta\,d\phi\,dr$$

Performing the integrations over angles, the final result is

$$I^{nlm}(P,\theta_p)=\sqrt{\frac{4\pi(2l+1)(l-m)!}{(l+m)!}}\,P_l^{|m|}(\cos\theta_p)\int_0^{\infty}R_{nl}(r)\,j_l(Pr)\,r^2\,dr \qquad 14$$

If the radial wavefunctions are assumed to have hydrogen atom-like form, then

$$R_{nl}(r)=e^{-r\sqrt{\frac{-2\mu E_{nl}}{\hbar^2}}}\sum_{i=0}^{\infty}D_{nl}^{i}\,r^{l+i} \qquad 15$$

where μ is the effective mass of the electron, E_{nl} is the state energy, and the coefficients, D_{nl}^{i} are set to give the best fit to the currently accepted radial wavefunctions for the atomic state in question. Equation 15 can then be substituted into Eq. 14 to yield the required I^{nlm} (see appendix A for the first few coefficients).

Part B - Evaluation of Screening Matrix Elements

A typical screening matrix element is of the form

$$M.E.^{s} = \langle P_1(\underline{r}') | \langle P_2(\underline{r}) | 1/|\underline{r}-\underline{r}'| \, | P_3(\underline{r}) \rangle | P_4(\underline{r}') \rangle$$

Taking the Fourier transform gives

$$\int d\underline{P}_1 d\underline{P}_2 d\underline{P}_3 d\underline{P}_4 C_1^*(\underline{P}_1) C_2^*(\underline{P}_2) C_3(\underline{P}_3) C_4(\underline{P}_4) \iint \frac{d\underline{r}\, d\underline{r}'\, e^{i(\underline{P}_1-\underline{P}_4)\cdot r'}}{|\underline{r}-\underline{r}'|\, e^{i(\underline{P}_3-\underline{P}_2)\cdot \underline{r}}} \quad 16$$

Letting $\underline{R} = \underline{r} - \underline{r}'$ yields

$$M.E.^{s} = \int d\underline{P}_1 d\underline{P}_2 d\underline{P}_3 d\underline{P}_4 C_1^*(\underline{P}_1) C_2^*(\underline{P}_2) C_3(\underline{P}_3) C_4(\underline{P}_4) \times \quad 17$$

$$\iint \frac{d\underline{r}\, d\underline{R}}{R} e^{i(\underline{P}_1-\underline{P}_4)\cdot \underline{R}} \, e^{i(\underline{P}_1+\underline{P}_2-\underline{P}_3-\underline{P}_4)\cdot \underline{r}}$$

Performing the integrations over $\underline{r}$ and $\underline{R}$ gives

$$M.E.^{s} = 4\pi(2\pi)^3 \int \frac{d\underline{P}_1 d\underline{P}_2 d\underline{P}\, C_1^*(\underline{P}_1) C_2^*(\underline{P}_2) C_3(\underline{P}_2+\underline{P}) C_4(\underline{P}_1-\underline{P})}{P^2} \quad 18$$

where $$P = |\underline{P}_3 - \underline{P}_2| .$$

Transforming the integrals to sums, the final result yields

$$ME^S = \frac{4\pi(2\pi)^{12}}{V^3} \sum_{\underline{P}_1, \underline{P}_2, \underline{P}} \frac{C_1^*(\underline{P}_1)\, C_2^*(\underline{P}_2)\, C_3(\underline{P}_2 + \underline{P})\, C_4(\underline{P}_1 - \underline{P})}{P^2} \qquad 19$$

Part C - Evaluation of the Ionic Matrix Elements

The ionic matrix element is of the type

$$M.E.^I = \langle \underline{P}_1(\underline{r}) | \nabla V(r) | \underline{P}_2(\underline{r}) \rangle$$

Taking the Fourier transform gives

$$M.E.^I = \int d\underline{P}_1\, d\underline{P}_2\, C_1(\underline{P}_1)\, C_2^*(\underline{P}_2) \int e^{i\underline{P}_1 \cdot \underline{r}}\, \nabla V(r)\, e^{-i\underline{P}_2 \cdot \underline{r}}\, d\underline{r} \qquad 20$$

Let $V(r)$ be spherically symmetric and of the following form

$$V(r) = \frac{e^2}{r} \left\{ Z_c e^{-Er} \left(1 + \sum_{n=1}^{\infty} a_n r^n\right) + (Z - Z_c) \right\} \qquad 21$$

where Z_c is the number of electrons in the ion core and, thus $Z - Z_c$ is the positive charge of the ions in the metal. The coefficients a_n and E are set to best represent the experimental ionic potential. Substituting the gradient of Eq. 21 into Eq. 20 and transforming integrals to sums yields

$$M.E.^{I} = \frac{N(2\pi)^6 e^2}{V^2} \sum_{\underline{P}_1,\underline{P}_2} C_1(\underline{P}_1)C_2^*(\underline{P}_2)\times \qquad 22$$

$$\int e^{i(\underline{P}_1-\underline{P}_2)\cdot\underline{r}}\left\{Z_c e^{-Er}/\left(1+\sum_{n=1}^{\infty}a_n r^n\right)+(Z-Z_c)\right\}d\underline{r}$$

Letting $(\underline{P}_1-\underline{P}_2)\cdot\underline{r} = |\underline{P}_1-\underline{P}_2|\,r\cos\theta$
and performing the integration over r gives

$$M.E.^{I} = \frac{2iNe^2(2\pi)^7}{V^2}\sum_{\underline{P}_1,\underline{P}_2} C_1(\underline{P}_1)\,C_2(\underline{P}_2)\times$$

$$\left[\frac{\pi(Z-Z_c)}{2|\underline{P}_1-\underline{P}_2|} + \frac{Z_c\tan^{-1}\left(E/|\underline{P}_1-\underline{P}_2|\right)}{|\underline{P}_1-\underline{P}_2|} +\right.$$

$$\frac{i\ Z_c}{2|\underline{P}_1-\underline{P}_2|}\sum_{j=1}^{\infty}\frac{(j-1)!\,a_j}{(E^2-|\underline{P}_1-\underline{P}_2|^2)^j}\left\{\left(E-i|\underline{P}_1-\underline{P}_2|\right)^j-\left(E+i|\underline{P}_1-\underline{P}_2|\right)^j\right\}\Bigg] \qquad 23$$

In practice, an infinite number of coefficients need not be used in R_{nl} and $V(r)$. However, a sufficient number should be determined to insure the desired accuracy.

CHAPTER VI

THEORETICAL INVESTIGATION OF SUPERCONDUCTING TANTALUM AND TUNGSTEN

In an earlier discussion of group V and group VI B.C.C. transition metals it was noted that these two similar periodic groups had very contrasting properties as superconductors. Thus, it would be appropriate to investigate both groups with the theoretical apparatus developed earlier in hope of finding some reasonable explanation. Tantalum and tungsten are chosen since experimental data is more readily available for these two metals. The calculations should emphasize differences between tantalum and tungsten consistent with being kept as simple as possible.

The first step is to reduce the expression for the electron-phonon coupling constant to a more soluble form. For a single band, the real part of the electron-phonon coupling constant is

$$\bar{g}_{\underline{k},\underline{k}+\underline{q}+\underline{G}_n,\alpha} = -\sqrt{\frac{\hbar N}{2M\omega_{\underline{q}\alpha}}}\,\underline{\epsilon}_{\underline{q}\alpha}\cdot\langle\underline{k}|\nabla V(r)|\underline{k}+\underline{q}+\underline{G}_n\rangle$$

$$+4\pi e^2\sum_{m}(\underline{k}')\frac{\bar{g}_{\underline{k}',\underline{k}'+\underline{q}+\underline{G}_m,\alpha}}{\Omega^2 V}\times$$

$$
\begin{aligned}
&\Bigg[\left\{\frac{1}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\right\}\times\\
&\qquad\Big\{\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle\\
&\qquad-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'+\underline{q}+\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\\
&\qquad+\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'+\underline{q}+\underline{G}_m\rangle|\underline{k}\rangle\\
&\qquad-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'+\underline{q}+\underline{G}_m\rangle\Big\}\\
&+\left\{\frac{1}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right\}\times\\
&\qquad\Big\{\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}'\rangle|\underline{k}\rangle\\
&\qquad-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'-\underline{q}-\underline{G}_m|R^{-1}|\underline{k}\rangle|\underline{k}'\rangle\\
&\qquad+\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}'-\underline{q}-\underline{G}_m\rangle|\underline{k}\rangle\\
&\qquad-\langle\underline{k}+\underline{q}+\underline{G}_n|\langle\underline{k}'|R^{-1}|\underline{k}\rangle|\underline{k}'-\underline{q}-\underline{G}_m\rangle\Big\}\Bigg]
\end{aligned}
\tag{1}
$$

Where Ω is the volume of the unit cell and the sums are over all occupied states. Substituting in the correct expressions for the matrix elements from chapter V and using

$$C_{\underline{k}}(\underline{P}) = \frac{N^{1/2}\,\delta_{\underline{P},-\underline{k}}}{(2\pi)^3}\; I(P,\theta_p) \qquad 2$$

gives

$$\bar{\delta}_{\underline{k},\underline{k}+\underline{q}+\underline{G}_n,\alpha} = -\sqrt{\frac{\hbar\; N}{2M\omega_{\underline{q}\alpha}}}\,\epsilon_{\underline{q}\alpha}\cdot\langle \underline{k}|\nabla V(r)|\underline{k}+\underline{q}+\underline{G}_n\rangle$$

$$+4\pi e^2 \sum_m (\underline{k}')\,\frac{\bar{\delta}_{\underline{k}',\underline{k}'+\underline{q}+\underline{G}_n\alpha}}{\Omega^2 V}\times$$

$$\Bigg[\left\{\frac{1}{E(\underline{k}')-E(\underline{k}'+\underline{q}+\underline{G}_m)}\right\}\times$$

$$\Bigg\{2I(\underline{k}+\underline{q}+\underline{G}_n)I(\underline{k}')I(\underline{k}'+\underline{q}+\underline{G}_m)I(\underline{k})\,\delta_{\underline{G}_m,\underline{G}_n}\frac{1}{|\underline{q}+\underline{G}_n|^2}$$

$$-I(\underline{k}+\underline{q}+\underline{G}_n)I(\underline{k}')I(\underline{k})I(\underline{k}'+\underline{q}+\underline{G}_m)\,\delta_{\underline{G}_n,\underline{G}_m}\frac{1}{|\underline{k}'-\underline{k}+\underline{G}_m-\underline{G}_n|^2}\Bigg\}$$

$$+\left\{\frac{1}{E(\underline{k}')-E(\underline{k}'-\underline{q}-\underline{G}_m)}\right\}\times$$

$$
\begin{aligned}
&\Big\{ 2 I(\underline{k}+\underline{q}+\underline{G}_n) I(\underline{k}'-\underline{q}-\underline{G}_m) I(\underline{k}') I(\underline{k}) \delta_{\underline{G}_m,\underline{G}_n} \frac{1}{|\underline{q}+\underline{G}_n|^2} \\
&- I(\underline{k}+\underline{q}+\underline{G}_n) I(\underline{k}-\underline{q}-\underline{G}_m) I(\underline{k}) I(\underline{k}') \delta_{\underline{G}_m,\underline{G}_n} \frac{1}{|\underline{k}'-\underline{k}-\underline{G}_n-\underline{q}|^2} \Big\} \Big] .
\end{aligned} \tag{3}
$$

Equation 3 represents a Fredholm integral equation of the second kind. For the purpose of simplicity, the screened coupling, $\bar{g}$, will be assumed to depend only upon the initial and final momentum at the Fermi energy. Since the screening term is either less than or about the same magnitude as the unscreened term, the relatively small error that has been introduced should not have a devastating effect upon the accuracy of the calculation. The form of the actual wavefunctions, represented by the quantities $I(\cdots)$, will be approximated as in the free electron case. In this simplification the quantities $I(\cdots)$ are set equal to $\Omega^{1/2}$ due to the fact that they are normalized to the unit cell volume Ω. Thus taking the average over polarization, the electron-phonon coupling constant is reduced to

$$\bar{g}_{\underline{k},\underline{k}+\underline{q}+\underline{G}_n} = \Bigg[\cos\theta_{\underline{q}}\, g_{\underline{q}} + \frac{4\pi e^2}{V}\,\bar{g}_{\underline{k},\underline{k}+\underline{q}+\underline{G}_n} \times$$

$$\sum(\underline{k}')\frac{1}{E(\underline{k}'+\underline{q}+\underline{G}_n)-E(\underline{k})}\left\{\frac{4}{q^2}-\frac{1}{|\underline{k}-\underline{k}'|^2}-\frac{1}{|\underline{k}+\underline{q}+\underline{G}_n-\underline{k}'|}\right\}\Bigg] \qquad 4$$

where

$$g_{\underline{q}} = \sqrt{\frac{\hbar}{2NM\omega_{\underline{q}}}}\;\frac{4\pi e^2 i}{\Omega}\Bigg[\frac{\pi(Z-68)}{2q} + \frac{68\cot^{-1}(E/q)}{q}$$

$$+\frac{68i}{2q}\sum_{j=0}^{6}\frac{j!\,a_{j+1}}{(E^2+q^2)^{j+1}}\left\{(E-iq)^{j+1}-(E+iq)^{j+1}\right\}\Bigg]. \qquad 5$$

The factor 68 represents the number of core electrons in tantalum and tungsten and seven coefficients are sufficient to represent the ionic potential. Solving for the electron-phonon coupling constant explicitly and converting from summation to integration over the Fermi sphere, gives

$$\bar{\delta}_{k,k+q+G_n} = \frac{\cos\theta_q\,\delta_q}{1+\frac{e^2}{\pi^2}\int\frac{d\underline{k}'}{E(\underline{k}'+\underline{q}+\underline{G}_n)-E(\underline{k}')}\left\{\frac{4}{|\underline{q}+\underline{G}_n|^2}-\frac{1}{|\underline{k}-\underline{k}'|^2}-\frac{1}{|\underline{k}+\underline{q}+\underline{G}_n-\underline{k}'|^2}\right\}} \qquad 6$$

Where a factor of two is inserted before the integral to include electrons of both spins. Using $E(\underline{k}) \simeq \hbar^2 k^2/2m$, the integrals are performed (Appendix B) for the three terms in the integrand. Briefly, for the first term one finds

$$\frac{4}{|\underline{q}+\underline{G}_n|^2}\int\frac{d^3k'}{E(\underline{k}'+\underline{q}+\underline{G}_n)-E(\underline{k}')} =$$

$$\frac{8\pi m k_f}{\hbar^2|\underline{q}+\underline{G}_n|^2}\left\{\frac{1}{2}+\left(\frac{4k_f-|\underline{q}+\underline{G}_n|^2}{8|\underline{q}+\underline{G}_n|\,k_f}\right)\ln\left(\frac{2k_f+|\underline{q}+\underline{G}_n|}{2k_f-|\underline{q}+\underline{G}_n|}\right)\right\} \qquad 7$$

which is the classical Bardeen[31] result. The other two terms are due to exchange and each yield identical results which are equal to

$$\int_{2k_f}\frac{d^3k'}{E(\underline{k}'+\underline{q}+\underline{G}_n)-E(\underline{k}')}\left(\frac{1}{|\underline{k}-\underline{k}'|^2}\right)$$

$$=\frac{(2\pi)^3\rho(E_f)}{4|\underline{q}+\underline{G}_n|k_fV}\ln\left(\frac{2}{1-\cos 2(\sin^{-1}K_c/2k_f)}\right) \qquad 8$$

Where $\rho(E_f)$ is the density of states at the Fermi energy and K_c represents the correlation momentum. Such momentum represents a minimum scattering momentum associated with a correlation hole about each electron. Electrons at relatively large distances from each other are effectively screened so small momentum transfers do not take place between them. Substituting these integrals into Eq. 6 yields

$$\delta_{k_f,|\underline{q}+\underline{G}_n|}=\cos\theta_q\times\delta_q$$

$$\left[1+\frac{8e^2mk_f}{\hbar^2\pi|\underline{q}+\underline{G}_n|^2}\left\{\frac{1}{2}+\right.\right.$$

$$\left.\left.\left(\frac{4k_f^2-|\underline{q}+\underline{G}_n|^2}{8k_f|\underline{q}+\underline{G}_n|}\right)\ln\left(\frac{2k_f+|\underline{q}+\underline{G}_n|}{2k_f-|\underline{q}+\underline{G}_n|}\right)\right\}-\frac{8\pi e^2}{|\underline{q}+\underline{G}_n|k_f}\left(\frac{\rho(E_f)}{V}\right)\ln\left(\frac{2k_f}{K_c}\right)\right]^{-1} \qquad 9$$

for the electron-phonon coupling.

An expression for the superconducting transition temperature is derived using a technique similar to that used by Carbotte and Dynes[13]. The desired quantity is the coupling times density of states function which is

$$\alpha^2(\omega)F(\omega)=\frac{\rho(E_f)}{8\pi k_f^2 V}\sum_{\substack{n\\|\underline{q}+\underline{G}_n|<2k_f}}\int_{1BZ} d^3\underline{q}\,\left|\bar{g}_{k_f,|\underline{q}+\underline{G}_n|}\right|^2\cdot\frac{\delta(\nu_{\underline{q}}-\omega)}{q} \qquad 10$$

where the sum over modes of vibration is implied. A computer program developed by Gilat and Raubenheimer[39] provides

$$F(\omega)=\frac{1}{N}\int_{1BZ}\frac{d^3\underline{q}}{(2\pi)^3}\,\delta(\nu_{\underline{q}}-\omega) \qquad 11$$

in histogram form for the phonon density of states $F(\omega)\Delta\omega$. Comparing Eq. 11 with Eq. 10, one finds that, for each value of the phonon wavevector q, the proper value of $\alpha^2(\omega)$ must be computed for all possible umklapp processes and then multiplied by the number of states placed in each histogram channel for that particular q. Thus, the histogram will then reflect $\alpha^2(\omega)\ F(\omega)\ \Delta\omega$ for channel width $\Delta\omega$. The coupling factor for phonon wavevector q and the nth umklapp process is then

$$EPH=\frac{\pi^2 N\rho(E_f)}{|\underline{q}+G_n|\,k_f^2\,V}\left|\bar{g}_{k_f,|\underline{q}+\underline{G}_n|}\right|^2 \qquad 12$$

A computer subroutine, EPH, which calculates Eq. 12 is added to the Gilat and Raubenheimer program (see Appendix C). Another subroutine, SWEEP, which constructs the phonon density of states histogram, is modified to find the coupling factor for all umklapp processes involving phonon wavevector q. In the same subroutine, the number of states placed into each histogram channel, $F(\omega)\ \Delta\omega$, is then multiplied by EPH for all umklapp processes to construct a new histogram containing $\alpha^2(\omega)\ F(\omega)\ \Delta(\omega)$ in each channel. The main program then calculates

$$\lambda=2\int_0^{\omega_0}\frac{\alpha^2(\omega)F(\omega)\,d\omega}{\omega} \qquad 13$$

for comparison with McMillan[15] together with the transition temperature using

$$T_c = \frac{\Theta_D}{1.45} e^{-\left[\frac{1.04\,(1+\lambda)}{\lambda-\mu^*(1+.62\lambda)}\right]} \qquad 14$$

for strong coupled superconductors. The value of μ^* represents effects of electron-electron repulsion whose values are taken from McMillan. Plots of both $F(\omega)\,\Delta\omega$ and $\alpha^2(\omega)\,F(\omega)\,\Delta(\omega)$ are constructed and shown in Tables 6 through 9.

Two crucial quantities are K_f and K_c. Upon examination of calculations for K_c for sodium[40], one can reason that, for the greatly increased density of electrons in a transition metal, $K_c = K_f$ should be a fairly good approximation. On the other hand K_f is freely varied about its free electron value to see what results can occur. Since, for the case of a real metal, K_f changes from point to point on the Fermi surface. Other parameters utilized by the program are the Debye temperature θ_D, the interatomic force constants, and the coefficients for the functions representing the ionic potential. Such data is

Table 4. List of potential coefficients and force constants for tantalum.

Ionic Potential Coefficients and Density of States		Force Constants (dynes/cm)	
E	1.725×10^{9}	α_1	16983
a_1	-9.774×10^{-2}	β_1	11201
a_2	3.894×10^{10}	α_2	1182
a_3	-4.770×10^{20}	β_2	1483
a_4	3.008×10^{30}	α_3	3546
a_5	-1.069×10^{40}	β_3	-5427
a_6	2.227×10^{49}	γ_3	1943
a_7	-2.698×10^{58}	α_4	3577
		β_4	-718
		γ_4	-1728
$n(e_f)$	1.52×10^{34}	ϵ_4	983
		α_5	-493
		β_5	812
		α_6	-3705
		β_6	134
		α_7	558
		β_7	-237
		γ_7	106
		ϵ_7	-683

Table 5. List of potential coefficients and force constants for tungsten.

Ionic Potential Coefficients and Density of States		Force Constants (dynes/cm)	
E	1.780×10^{9}	α_1	23000
a_1	1.061×10^{-1}	β_1	19200
a_2	3.926×10^{10}	α_2	47300
a_3	-4.795×10^{20}	β_2	800
a_4	3.023×10^{30}	α_3	3200
a_5	-1.076×10^{40}	β_3	1400
a_6	2.248×10^{49}	γ_3	4900
a_7	-2.734×10^{58}		
$\rho(E)$	2.56×10^{33}		

summarized in tables 4 and 5.

The final results include Figs. 8 and 9 of which Fig. 9 agrees quite well with an experimental investigation by L. Y. L. Shen[41]. The dimensionless coupling parameter, λ, and the superconducting transition temperature stemming from it show reasonable values which upon freely varying K_f, can be made to agree with experimental values.

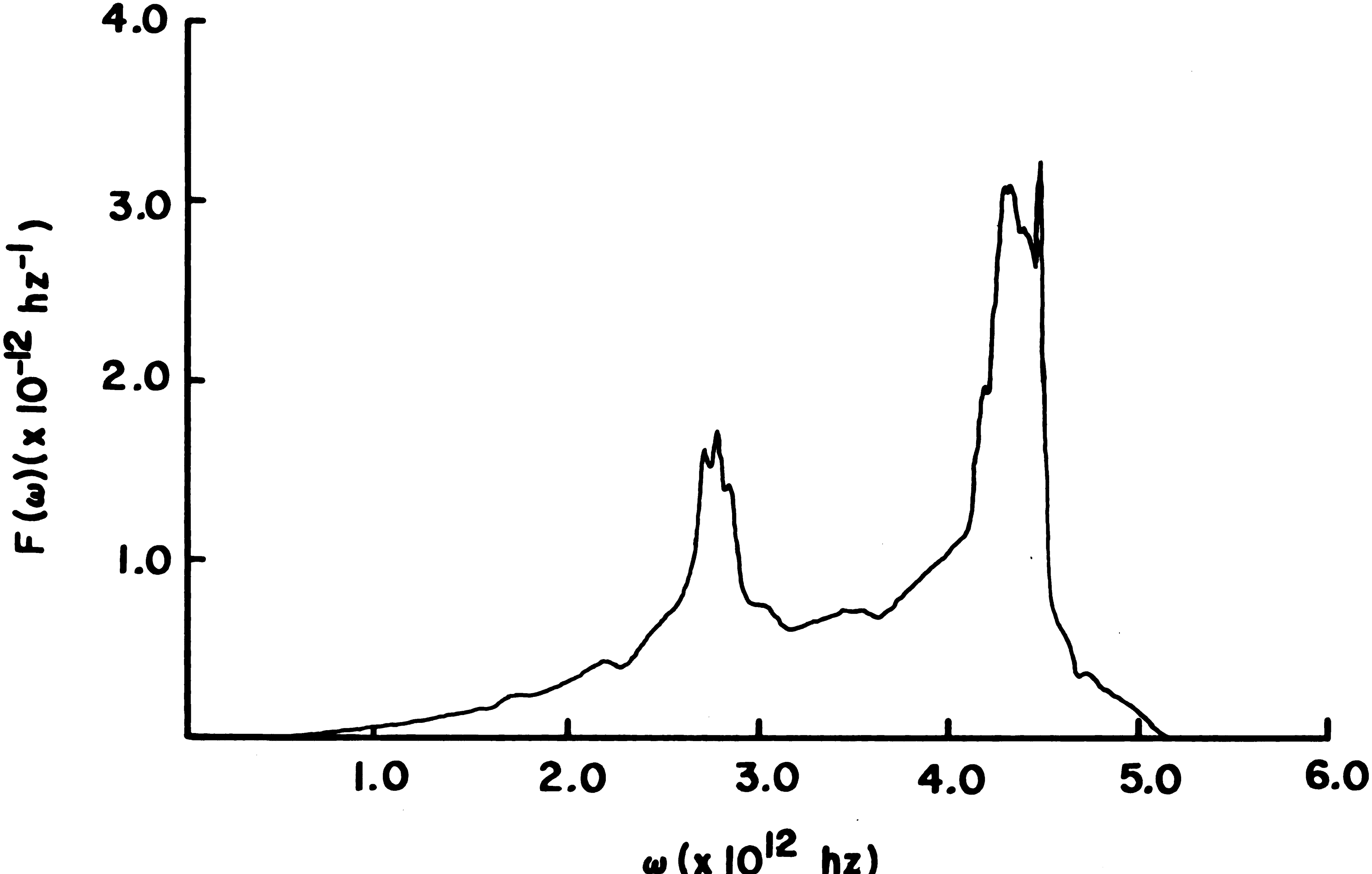

Figure 6. Density of phonon states for tantalum.

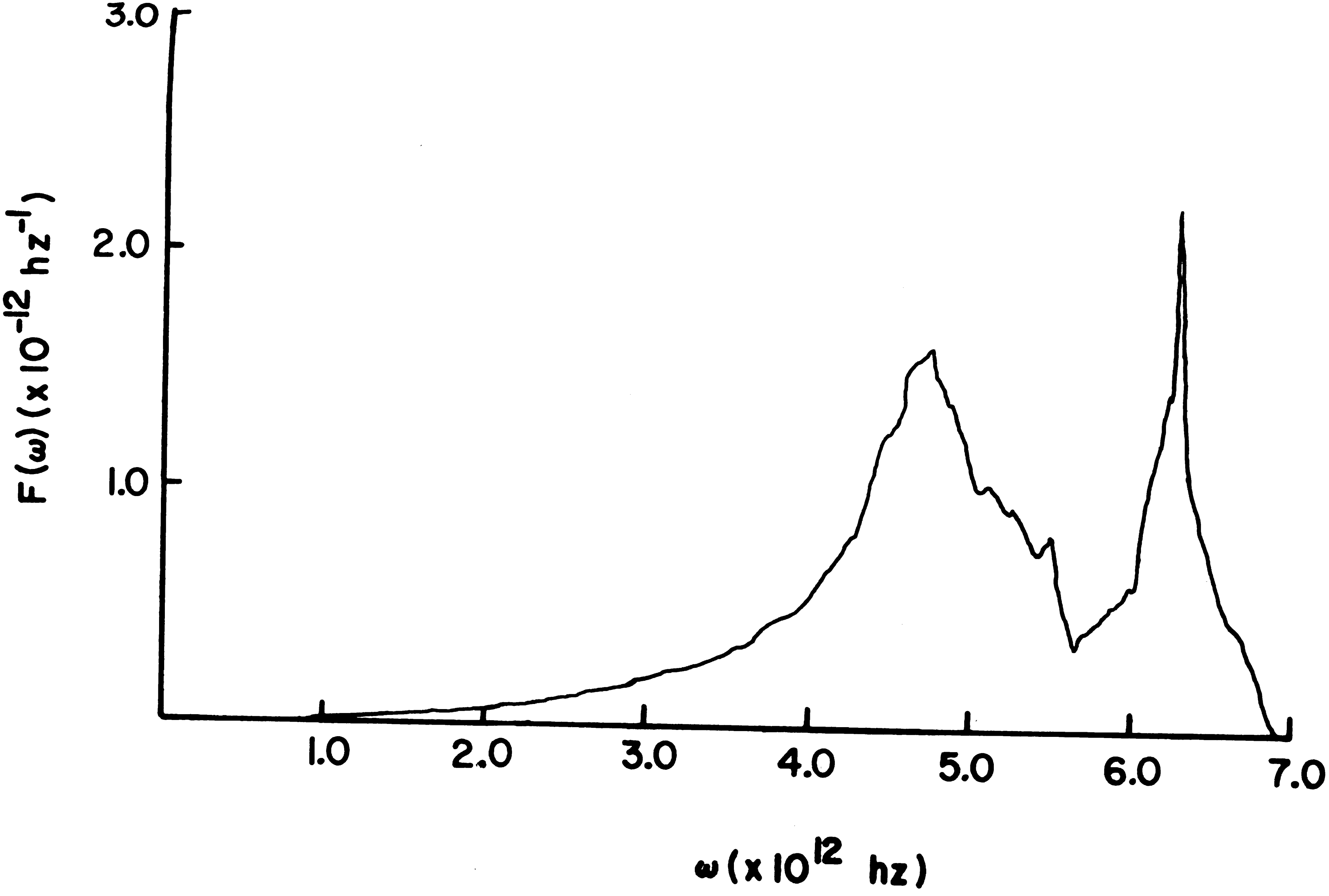

Figure 7. Density of phonon states for tungsten.

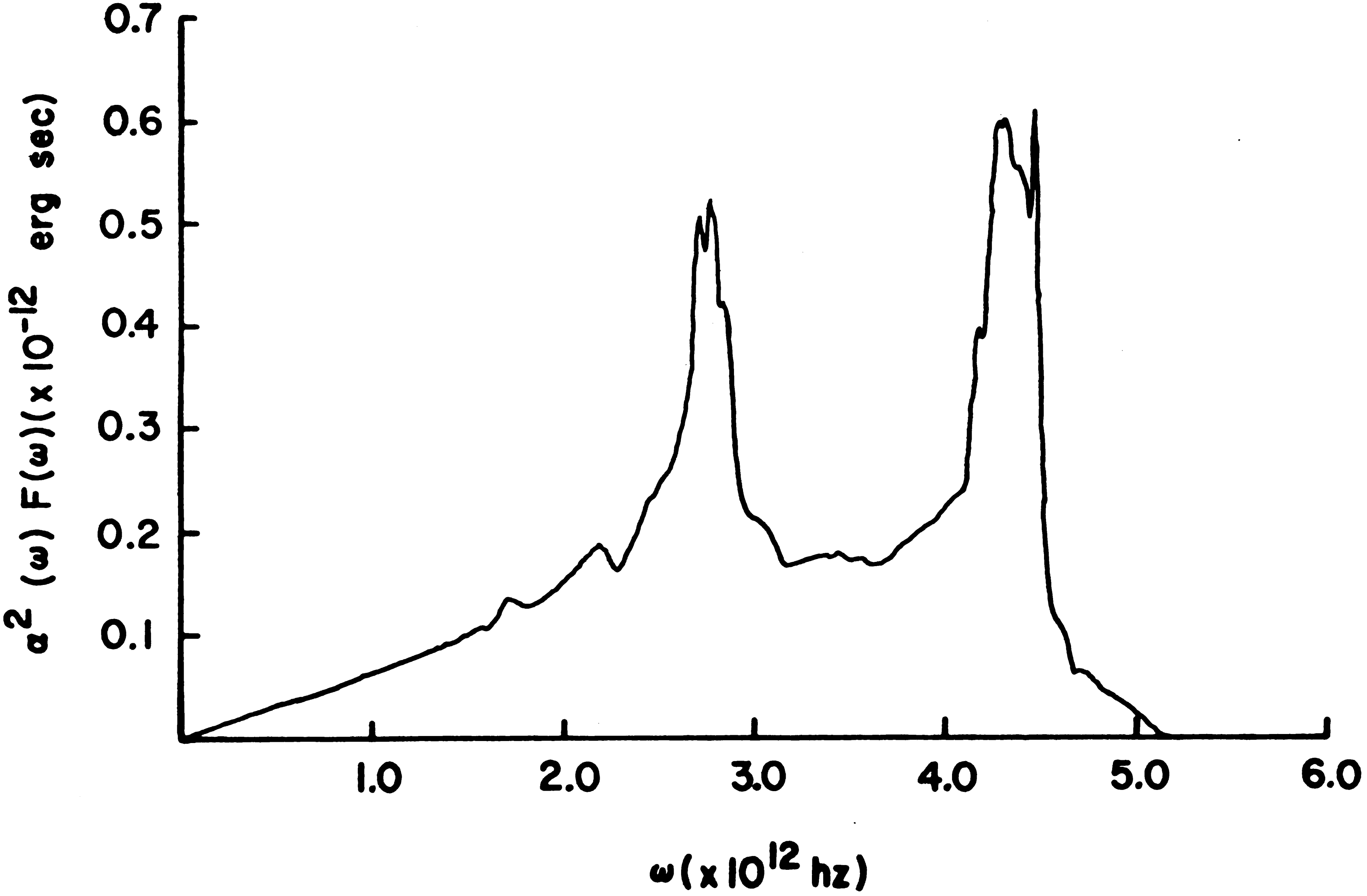

Figure 8, Coupling times density of states for tantalum,

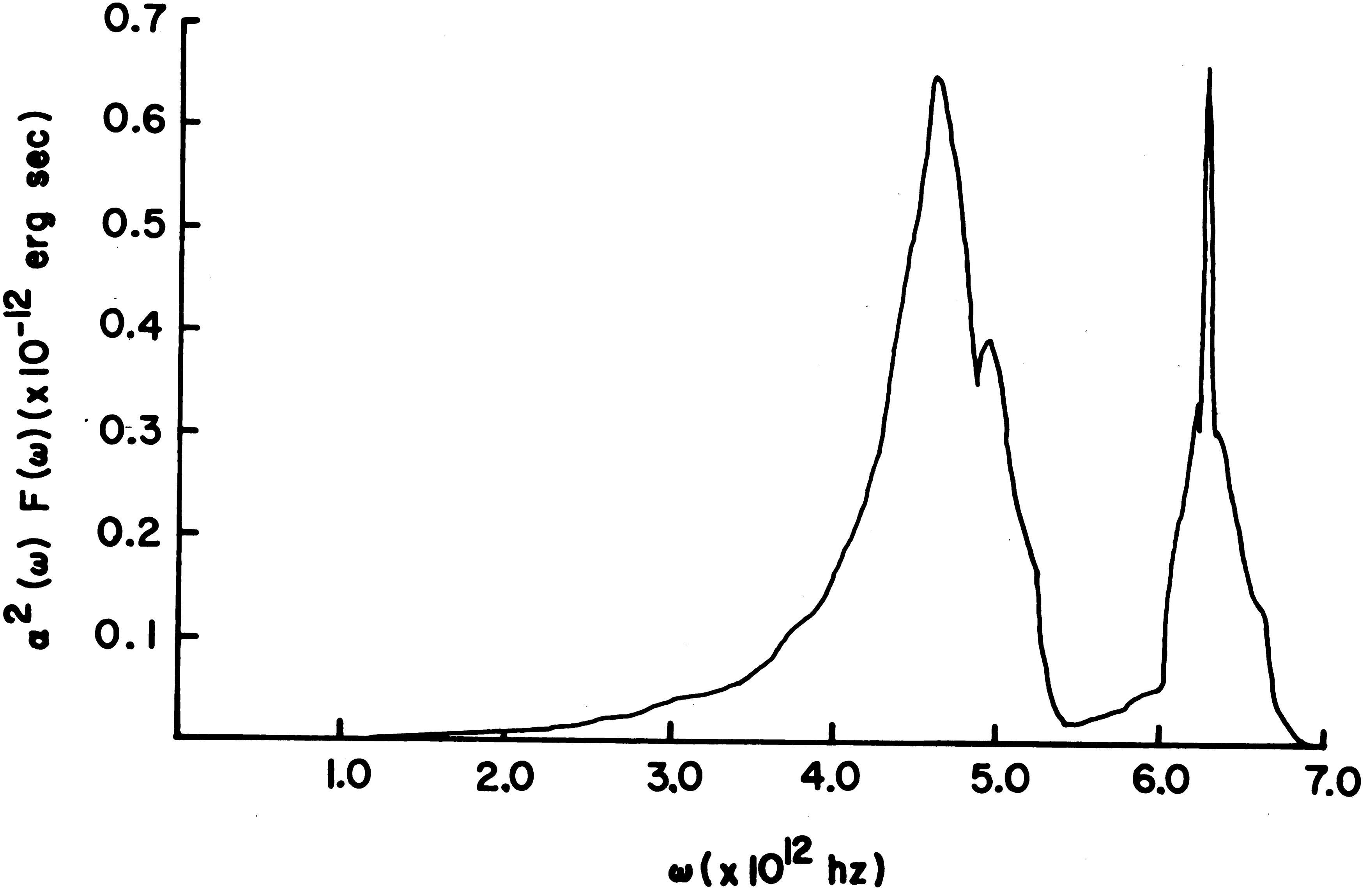

Figure 9. Coupling times density of states for tungsten.

CHAPTER VII

CONCLUSION

The objective of this research was to examine, theoretically, transition elements in order to determine whether or not their superconductivity is due to a phonon mediated interaction between electrons. The task was to find an expression for electron-phonon coupling from an appropriate model and, then, with the theoretical apparatus used by Carbotte and Dynes[13] for simple metals, find the superconducting properties of the transition metal in question. It may be recalled that all of the conduction electrons were assumed to lie in a single band similar to the free electron case. Although such simplifications cannot be expected to yield exact expressions, the results can, nevertheless, tell a great deal about the system at hand.

First to be considered are the coupling times phonon density of states curves for tantalum and tungsten (Figures 8 and 9). Comparing these two figures to the corresponding phonon densities of states shows about twice the effective coupling at lower (transverse) frequencies compared to that at the highest (longitudinal) frequencies for both metals. in the case of tantalum, the curves compare favorably with

Table 6. λ vs K_f for tantalum and tungsten.

Tantalum		Tungsten	
K_f ($\times 10^8$)	λ	K_f ($\times 10^8$)	λ
1.601	32.8	0.75	0.405
2.0	124.34	0.8	0.342
2.1	5.414	0.9	0.266
3.3	2.358	1.0	0.213
3.5	2.207	1.4	0.183
4.0	1.933	1.779	0.164
5.0	1.041	2.0	0.154
6.0	0.671		
$Tc=4.48^\circ K$	0.69	$T_c=0.012^\circ K$	0.29

experimental results obtained by L. Y. L. Shen[41]. Thus, it appears that the qualitative features of the theoretical screening are basically correct for tantalum. Moreover, treating all conduction electrons as members of a single band with no distinction for s-like or d-like states has not produced any serious difficulties.

The curves (Figures 10 and 11) giving the dimensionless coupling parameter, λ, versus the Fermi momentum K_f, require deeper interpretation. For tantalum it is apparent from the results that in the theory one must use a value of K_f about twice as large as would be expected for an electron gas of similar density (1.6×10^8 qm-cm/sec) to achieve the correct values of λ (0.69) and, hence, Tc (4.48°K). The situation with tungsten is somewhat reversed. Here the theory requires a value of K_f of about one half that expected in an electron gas of similar density (1.8×10^8 qm-cm/sec) to get the correct λ (0.29) and Tc (0.012°K). Thus, if the theory is essentially correct for group V transition metals like tantalum, then what properties of group VI transition metals such as tungsten prove to be incongruent with these calculations? It must be remembered that all electrons were assumed to be capable of pairing and no distinction was made between s-like and d-like carriers. One such interpretation is that the conduction electrons in tungsten do separate into both an

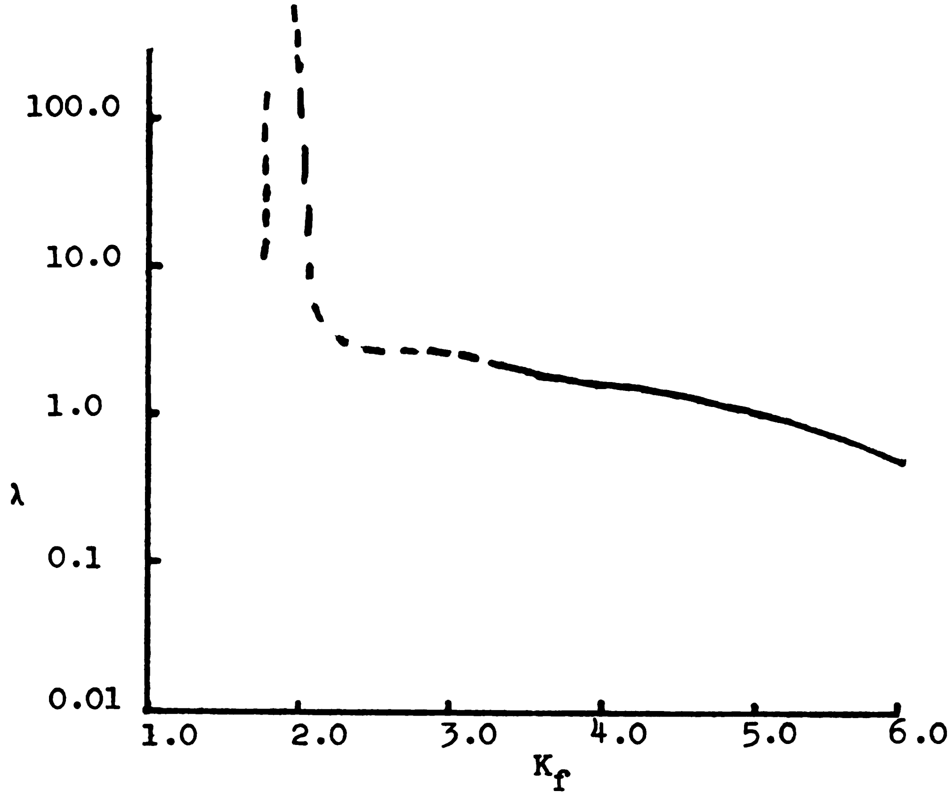

Figure 10. λ vs K_f for tantalum.

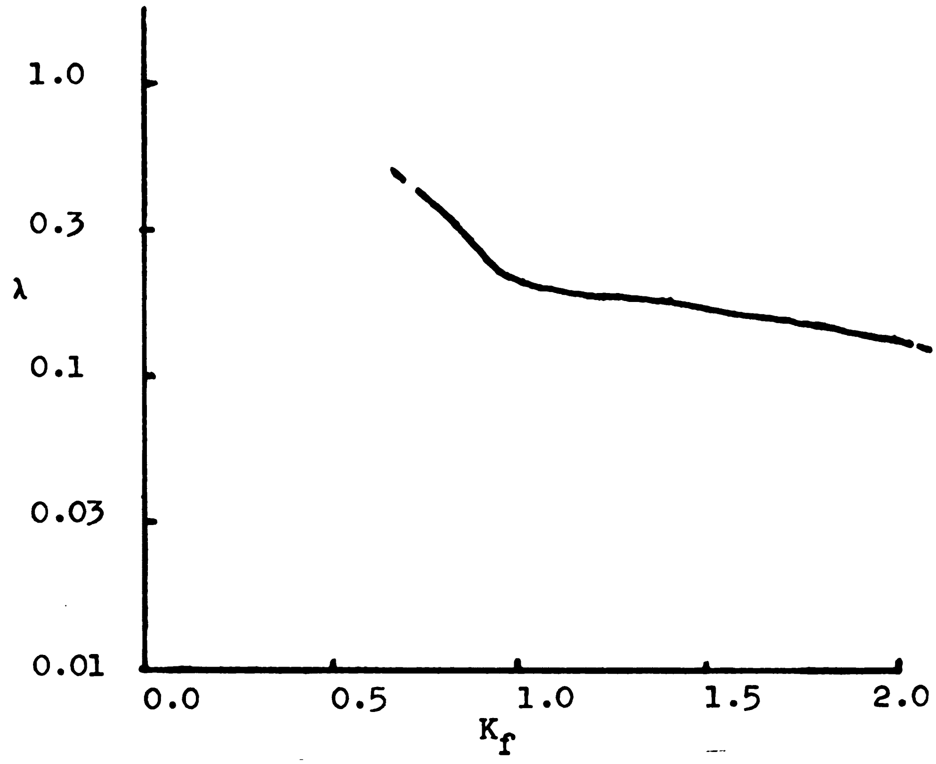

Figure 11. λ vs K_f for tungsten.

s-like and a d-like group. If only the more weakly coupled s-like electrons could form Cooper pairs then both the abnormally low value of K_f required in the theory and the low superconducting transition temperature can be justified. The assumption that the theory is correct for tantalum is supported, in addition to agreement with the Shen results, by reasoning that all of the conduction electrons can form Cooper pairs and that strong coupling results from the tendency of these electrons to form into a group of d-like electrons strongly correlated to the positions of the ions together with an itinerent s-like group.

In conclusion, a theoretical investigation of the superconducting properties of transition metals using the same phonon-mediated theory successful for simple metals has yielded credible results.

APPENDICES

APPENDIX A

EVALUATION OF I ^{nlm}

(1) 1 = 0 case

$$I^{n00}(P,\theta_p) = 2\sqrt{\pi}\int_0^\infty R_{n0}(r)\, j_0(Pr)\, r^2\, dr$$

$$= 2\sqrt{\pi}\int_0^\infty \left(e^{-r\sqrt{\frac{-2\mu E_{n0}}{\hbar^2}}} \sum_{i=0}^{\infty} D_{n0}^{i}\, r^{i} \times \right.$$

$$\left.\left(\frac{\sin Pr}{Pr}\right) r^2\, dr\right.$$

$$= \frac{2\sqrt{\pi}}{P}\sum_{i=0}^{\infty} D_{n0}^{i} \left\{\frac{(i+1)!}{\left(P^2 - \frac{2\mu E_{n0}}{\hbar^2}\right)^{\frac{i+2}{2}}} \times \right.$$

$$\left. \sin\left((i+2)\tan^{-1}\frac{\hbar P}{\sqrt{-2\mu E_{n0}}}\right)\right\}$$

$$I^{n00}_{(P,\theta_p)} = 2\sqrt{\pi}\sum_{i=0}^{\infty}\sum_{j=0}^{i+2}\left\{\frac{D^{i}_{n0}\,(i+1)!\,(i+2)!}{(i-j+2)!\;j!}\right\}\times$$

$$(-2\mu E_{n0})^{\frac{i-j+2}{2}}\left\{\frac{P^{j-1}}{\left(P^{2}-\frac{2\mu E_{n0}}{\hbar^{2}}\right)^{i+2}}\right\}$$

(2) 1 = 1 case

$$I^{n1m}(P,\theta_p)=2\sqrt{3\pi}\sqrt{\frac{(1-m)!}{(1+m)!}}\,P_{1}^{|m|}(\cos\theta_p)\times$$

$$\int_0^{\infty}R_{n1}(r)\,j_1(Pr)\,r^2\,dr$$

$$=2\sqrt{3\pi}\sqrt{\frac{(1-m)!}{(1+m)!}}\,P_{1}^{|m|}(\cos\theta_p)\sum_{i=0}^{\infty}D^{i}_{n1}\times$$

$$\left[\frac{1}{P^{2}}\int_0^{\infty}r^{i+1}e^{-r\sqrt{\frac{-2\mu E_{n1}}{\hbar^{2}}}}\sin pr\,dr-\frac{1}{P}\int_0^{\infty}r^{i+2}e^{-r\sqrt{\frac{-2\mu E_{n1}}{\hbar^{2}}}}\cos pr\,dr\right]$$

$$I^{n1m}_{(p,\theta_p)}=2\sqrt{\frac{3\pi\,(1-m)!}{(1+m)!}}\;P_1^{|m|}(\cos\theta_p)\sum_{i=0}^{\infty}D_{n1}^{i}\times$$

$$\left[\sum_{j=0}^{i+2}\left\{\frac{(i+1)!\,(i+2)!}{(i-j+2)!\;j!}\right\}\left\{\frac{i^{j-1}+(-i)^{j-1}}{2\hbar^{i+2-j}}\right\}(-2\mu E_{n1})^{\frac{i+2-j}{2}}\left\{\frac{p^{j-2}}{\left(p^2-\frac{2\mu E_{n1}}{\hbar^2}\right)^{i+2}}\right\}\right.$$

$$\left.-\sum_{j=0}^{i+3}\left\{\frac{(i+2)!(i+3)!}{(i-j+3)!\;j!}\right\}\left\{\frac{i^{j}+(-i)^{j}}{2\hbar^{i+3-j}}\right\}(-2\mu E_{n1})^{\frac{i+3-j}{2}}\left\{\frac{p^{j-1}}{\left(p^2-\frac{2\mu E_{n1}}{\hbar^2}\right)^{i+3}}\right\}\right]$$

(3) l = 2 case

$$I^{n2m}_{(p,\theta_p)}=2\sqrt{\frac{5\pi(2-m)!}{(2+m)!}}\;P_2^{|m|}(\cos\theta_p)\times$$

$$\int_0^{\infty}R_{n2}(r)\,j_2(pr)\,r^2dr$$

$$=2\sqrt{\frac{5\pi(2-m)!}{(2+m)!}}\;P_2^{|m|}(\cos\theta_p\sum_{i=0}^{\infty}D_{n2}^{i}\times$$

$$\left[\frac{3}{p^3}\int_0^{\infty}r^{i+1}e^{-r\sqrt{\frac{-2\mu E_{n2}}{\hbar^2}}}\sin pr\,dr\right.$$

$$-\frac{1}{p}\int_0^{\infty}r^{i+3}e^{-r\sqrt{\frac{-2\mu E_{n2}}{\hbar^2}}}\sin pr\,dr$$

$$\left.+\frac{3}{p^2}\int_0^{\infty}r^{i+2}e^{-r\sqrt{\frac{-2\mu E_{n2}}{\hbar^2}}}\cos pr\,dr\right]$$

$$I^{n2m}_{(P,\theta_P)} = 2\sqrt{\frac{5\pi(2-m)!}{(2+m)!}}\, P_2^{|m|}(\cos\theta_P)\sum_{i=0}^{\infty} D^{i}_{n2} \times$$

$$\left[\sum_{j=0}^{i+2}\left\{\frac{3(i+1)!\,(i+2)!}{(i-j+2)!\; j!}\right\}\left\{\frac{i^{j-1}+(-i)^{j-1}}{2\hbar^{i+2-j}}\right\}(-2\mu E_{n2})^{\frac{i+2-j}{2}}\left\{\frac{P^{j-3}}{\left(P^2-\frac{2\mu E_{n2}}{\hbar^2}\right)^{i+2}}\right\}\right.$$

$$-\sum_{j=0}^{i+4}\left\{\frac{(i+3)!\,(i+4)!}{(i-j+4)!\,j!}\right\}\left\{\frac{i^{j-1}+(-i)^{j-1}}{2\hbar^{i+4-j}}\right\}(2\mu E_{n2})^{\frac{i+4-j}{2}}\left\{\frac{P^{j-1}}{\left(P^2-\frac{2\mu E_{n2}}{\hbar^2}\right)^{i+4}}\right\}$$

$$\left.-\sum_{j=0}^{i+3}\left\{\frac{3(i+2)!\,(i+3)!}{(i-j+3)!\; j!}\right\}\left\{\frac{i^{j}+(-i)^{j}}{2\hbar^{i+3-j}}\right\}(-2\mu E_{n2})^{\frac{i+3-j}{2}}\left\{\frac{P^{j-2}}{\left(P^2-\frac{2\mu E_{n2}}{\hbar^2}\right)^{i+3}}\right\}\right]$$

APPENDIX B

EVALUATION OF INTEGRALS

Part- I Exchange Screening

$$\frac{\rho(E_{k'})}{V} = \frac{4\pi k'^2}{\frac{dE_{k}}{dk}}$$ with $E_{k'}$, as a function of scalar k'only

Thus, using

$$E(\underline{k}'+\underline{q})-E(k') \cong \frac{dE_{k'}}{dk'} \sin\Theta_{\nabla_{\underline{k}}E,q}\, q$$

and

$$\sin\Theta_{\nabla_{\underline{k}}E,q} = \frac{\Delta k'}{k'}$$

Where due to the fact $|\underline{k}-\underline{k}'|$ is small only near the Fermi surface, $\Delta k'$ is the effective range of k' for non zero integrand. Then,

$$\int \frac{d^3k'}{E(\underline{k}'+\underline{q})-E(\underline{k}')} \frac{1}{|\underline{k}-\underline{k}'|^2}$$ becomes

$$\int \frac{d^3 k'}{E(\underline{k}'+\underline{q})-E(\underline{k}')} \frac{1}{|\underline{k}-\underline{k}'|^2}$$

$$= \int \frac{k'^2 dk' \sin\theta \, d\theta \, d\phi}{\left(\frac{4\pi q V k'^2 \sin\theta_{\nabla E, q}}{(2\pi)^3 \rho(E_{k'})} \right)} \frac{1}{(k^2 + k'^2 - 2kk'\cos\theta)}$$

$$= \frac{(2\pi)^3 k \rho(E_{k'})}{4\pi q V \Delta k'} \int_{\Delta k'} \int_{\theta_0}^{\pi} \int_{0}^{2\pi} \frac{dk' \, d\theta \, d\phi \, \sin\theta}{k^2 + k'^2 - 2kk'\cos\theta} .$$

over the range of integration k' = k,

$$= \frac{(2\pi)^3 \rho(E_k)}{4 q V k} \int_{\theta_0}^{\pi} \frac{\sin\theta \, d\theta}{(1-\cos\theta)}$$

$$= \frac{(2\pi)^3 \rho(E_k)}{4 q k \; V} \ln(1-\cos\theta) \Big|_{\theta_0}^{\pi}$$

$$= \frac{(2\pi)^3 \rho(E_k)}{4 q k \; V} \ln\left(\frac{2}{1-\cos\theta_0} \right)$$

Finally,

$$\int \frac{d^3k'}{E(\underline{k}'+q)-E(k')}\,\frac{1}{|k-k'|} =$$

$$\frac{(2\pi)^3\rho(E_f)}{2qVk_f}\ln\left(\frac{2}{1-\cos 2(\sin^{-1}K_c/2K_f)}\right)$$

Where the correlation hole, K_c is given by

$$\Theta_0 \cong \sin^{-1}(K_c\backslash 2K_f)$$

Part- II Normal Screening

$$\int \frac{d^3k'}{E(\underline{k}'-\underline{q})-E(\underline{k}')}\,\frac{4}{q^2}$$

Using cylindrical coordinates take 3 axis $\parallel$ to q and $E(\underline{k})=\frac{\hbar^2 k^2}{2m}$.

$$=\frac{4}{q^2}\left(\frac{2m}{\hbar^2}\right)\int\frac{\rho\,d\rho\,d\theta\,dz}{(z+q)^2+\rho^2-(\rho^2+z^2)}$$

$$=\frac{8m(2\pi)}{\hbar^2 q^2}\int\frac{dz}{(z+q)^2-z^2}\int_0^{(k_f^2-z^2)^{1/2}}\rho\,d\rho$$

$$=\frac{16\pi m}{\hbar^2 q^2}\left(\frac{1}{2}\right)\int\frac{dz\,(k_f^2-z^2)}{(z+q)^2-z^2}$$

$$=\frac{8\pi m}{\hbar^2 q^2}\lim_{\epsilon\to 0}\left\{\int_{-k_f}^{-\frac{q}{2}-\epsilon}\frac{dz\,(k_f^2-z^2)}{(z+q)^2-z^2}\right.$$

$$\int_{-\frac{q}{2}-\epsilon}^{k_f}\frac{dz\,(k_f^2-z^2)}{(z+q)^2-z^2}$$

$$=\frac{8\pi m}{\hbar^2 q^2}\lim_{\epsilon\to 0}\left[\left(\frac{4qk_f-q^3}{16q^3}\right)\ln u+\frac{u}{4q}-\frac{u^2}{16q^3}\right]\Bigg|_{-2qk_f+q^2}^{-\epsilon}\Bigg|_{\epsilon}^{2qk_f+q^2}$$

$$\int \frac{d^3k'}{E(\underline{k}'+\underline{q})-E(\underline{k}')}\frac{4}{q^2}=\frac{8\pi m}{\hbar^2 q^2}\left\{\frac{4k_f^2-q^2}{8q}\ln\left(\frac{2k_f+q}{2k_f-q}\right)\right.$$

$$\left.+\frac{4qk_f}{4q}+\frac{(-2qk_f+q^2)^2-(2qk_f+q^2)^2}{16q^3}\right\}$$

$$=\frac{8\pi m}{\hbar^2 q^2}\left\{\frac{4k_f^2-q^2}{8q}\ln\left(\frac{2k_f+q}{2k_f-q}\right)+k_f-\frac{k_f}{2}\right\}$$

$$=\frac{8\pi m k_f}{\hbar^2 q^2}\left\{\frac{1}{2}+\left(\frac{4k_f^2-q^2}{8qk_f}\right)\ln\left(\frac{2k_f+q}{2k_f-q}\right)\right\}$$

APPENDIX C

```
C REVISED VERSION OF GILAT AND RAUBENHEIMER PROGRAM G(NU) TO INCLUDE
C A FACTOR GIVING ELECTRON-ION COUPLING. UMKLAPP PROCESSES ARE INCLUDED.
```

```
      PROGRAM GNU
      DIMENSION CTA(1500),CTC(1500),TITLE(16)
      DIMENSION AL(3),Q(3),V(12),GD1(12),GD2(12),GD3(12),PX(80)              4
      DIMENSION AMAS(12)                                                     5
      DIMENSION FV(12,12)                                                    6
      DIMENSION POTEN(7),CTI(1500)                                          6A
      COMMON/X2/ANN                                                          7
      COMMON/X3/PI,CPT,PX,U,SC,NSFB,AMAS,DQ                                  8
      COMMON/X4/FV,V                                                         9
      COMMON/X5/LA,CTA,DVA,AHALF,VOLUME,ASQ,NPRINT,XM                       10
      COMMON/X6/KM,KK,I, J,K                                                11
      COMMON/X7/NNN                                                         12
      COMMON/X8/ALP,EKF,RHO,EP,Z,POTEN,CTI,AMASS,OMEGA                     12A
C                                                                           13
C  THE ONLY (DIMENSIONED) ARRAYS IN COMMON STATEMENTS ARE CTA(7000),        14
C  FV(12,12) AND V(12) .  V IN GNU IS EQUIVALENT TO PH IN SURR. FREQ        15
C                                                                           16
 7102 FORMAT(5X,22HFREQ. CHANNEL WIDTH =  ,F9.6  )
  101 FORMAT(1H- )
  105 FORMAT(1X,I4,3I3,2X,3HU =,F4.1,5X,3HQ =,3F9.5,5X,3HV =,6F9.5)         19
  106 FORMAT(1H1,10X, 22HARRAY OF G(NU)/(NU)**2  ///)
  107 FORMAT(1X,I5,3I3,F5.1,4X,6F9.5/8F9.5)                                 21
 1121 FORMAT (10X, I5)
 2107 FORMAT(4F20.6)                                                        22
 2177 FORMAT(4F20.6)
  108 FORMAT(1H0,10X,18HATOMIC MASS(ES) =  ,4F10.4 )                        23
```

```
 2109 FORMAT(16H0FORCE CONSTANTS  )                                        24
 1111 FORMAT(33H    (NSER, NNN, KK, IMIN, IMAX) =  ,10I4)
 1112 FORMAT(44H0     CYCLE NO., KK, NO. CUBES, IMIN, IMAX =  ,10I5)      26
  119 FORMAT(8F10.5)
 1120 FORMAT(20I5)                                                         28
 2120 FORMAT(1H0, 10F11.4)                                                 29
  123 FORMAT(16A5)
 8123 FORMAT(18H FREQ(10**12 CPS), ,20X, 24HG(NU) HISTOGRAM CHANNELS //) 31
 9123 FORMAT(1H1,10X,16A5/1H-)
  124 FORMAT  (2I5, 7F10.0)
  126 FORMAT (2F10.5, 2I5)
  125 FORMAT(10F8.0)                                                       33
 9125 FORMAT(5F16.8)                                                       34
 9126 FORMAT (1H1/21H DEGREES OF FREEDOM =  ,F10.4)                       34A
 9127 FORMAT (1H1/09H LAMBDA =  ,F10.4)                                   34B
 9128 FORMAT (1H1/25H TRANSITION TEMPERATURE =  ,F10.4)                   34C
 1002 FORMAT(1H1)                                                          35
 1003 FORMAT(1H1/35H      *NEGATIVE* FREQUENCY CHANNELS  /1H-)
 2000 FORMAT (10X, 15H EIGENVECTORS    )
 2001 FORMAT (10X, 9HV(1) = ( , 3F15.6, 1H) )
 2002 FORMAT (10X, 9HV(2) = ( , 3F15.6, 1H) )
 2003 FORMAT (10X, 9HV(3) = ( , 3F15.6, 1H) )
 9944 FORMAT (F20.6,3F20.6)
C  ALL *LOGICAL IF* STATEMENTS HAVE BEEN REPLACED BY ARITHMETIC IF*S      38
C  SOME LOGICAL IFS HAVE BEEN LEFT IN AS COMMENTS, INDICATED BY C*        39
C                                                                          40
C  ACTIVATE PLOTTING ROUTINES FIRST                                        41
C                                                                          43
C  NDIMA AND NDIMC ARE THE DIMENSIONS OF CTA AND CTC                       44
      NDIMA=1500
      NDIMC = NDIMA                                                        46
C                                                                          47
C  READ IDENTIFICATION NUMBER  ( 5 DIGITS)
      READ 1120, IDENT
      PRINT 1121, IDENT
```

```
C READ 1ST DATA CARD
      READ 123, TITLE
      PRINT 123, TITLE
C
C READ 2ND DATA CARD
      READ 1120, NSFR, NNN, NFC
      PRINT 1120, NSFR, NNN, NFC
C  NSFR = 1 FOR SIMPLE CUBE,  =2 FOR FCC  AND =3 FOR BCC .
C  NNN = DIMENSION  ( =3 TIMES NO. OF ATOMS/UNIT CELL )
C  NFC = NO. OF FORCE CONSTANTS TO BE READ IN FURTHER ON .
C
C READ 3RD DATA CARD
      READ 119, DVA, XM, DQ
      PRINT 119, DVA, XM, DQ
C  DVA = CHANNEL WIDTH OF HISTOGRAM (IN 10**12 C/S)
C  XM = MAX FREQ  (UNITS OF 10**12 C/S)
C  DQ = DELTA Q FOR COMPUTING GRAD(NU), USUALLY DQ = 0.0001
C
C READ 4TH DATA CARD
      READ 119, AMAS(1), AMAS(4), AMAS(7), AMAS(10)
      PRINT 119, AMAS(1), AMAS(4), AMAS(7), AMAS(10)
C
C READ 5TH DATA CARD(S) - FORCE CONSTANTS
      READ 2107, (PX (I), I=1, NFC)
      PRINT 2107, (PX (I), I=1, NFC)
C
      L = NFC + 1
      DO 527 J=L,80
  527 PX(J) = 0.0
C
C READ 6TH DATA CARD
      READ 1120, NCTA,NCTC,NTAPE,NPLOT,KK,KG,IMIN,IMAX,NPCH,NPRINT
      PRINT 1120,NCTA,NCTC,NTAPE,NPLOT,KK,KG,IMIN,IMAX,NPCH,NPRINT
C
      READ 119,POTEN(1),POTEN(2),POTEN(3),POTEN(4),POTEN(5),POTEN(6),
```

```
     1POTEN(7),FP                                                       76A
      READ 119,AMASS,OMEGA,Z,RHO,ALP,FLE,THETA                          77A
      READ 119,FKF
  710 PRINT 9123, TITLE
      PRINT 108, AMAS(1), AMAS(4), AMAS(7), AMAS(10)
      WRITE (61, 2109)
      PRINT 2107, (PX(I), I=1, NFC)
      PRINT 2177,(POTEN(I),I=1,4)                                       XXXXXXXX
      PRINT 2177,(POTEN(I),I=5,7),FP                                    XXXXXXXX
      PRINT 2177,AMASS,OMEGA,Z,RHO                                      XXXXXXXX
      PRINT 2177,ALP,FLE,THETA,FKF                                      XXXXXXXX
  310 LA = XM/DVA + 51.0                                                88
C  WE START STORING G(NU) IN LOC. 51 OF CTA IN CASE OF *NEG* FREQS      89
      NS = 0                                                            90
C  NS IS TO BE THE MESH POINT SEQUENCE NUMBER                           91
C FIND SOME CONVENIENT CONSTANTS ETC. WITH SUBROUTINE CONST .           92
C                                                                       93
      AMASS=AMASS*1.66043E-24
      CALL CONST                                                        94
C                                                                       95
      DO 10 I = 1,NDIMA                                                 96
      CTT(I)=0.0                                                        96A
   10 CTA(I) = 0.0                                                      97
      DO 406 M = 1,NDIMC                                                98
  406 CTC(M) = 0.0                                                      99
C                                                                       100
  311 GO TO (312,313,314),NSER                                          101
  312 JTMAX = KK                                                        102
      PP = 0.5                                                          103
      GO TO 320                                                         104
  313 JTMAX = 4*KK                                                      105
      PP = 1.0                                                          106
      GO TO 320                                                         107
  314 JTMAX = 2*KK                                                      108
      PP = 1.0                                                          109
```

```
  320 XJTMAX=JTMAX
      CUBE=PP/XJTMAX
      IF(IMAX)1320,1320,2320
 1320 IMAX = JTMAX
 2320 IF(IMIN)321,321,401
  321 IMIN = 3
  401 PRINT 1111, NSFR, NNN, KK, IMIN, IMAX
      PRINT 101
C
C  BRILLOUIN ZONE NOW BROKEN UP INTO THREE PARTS (KM = 1,3)
C
      DO 69 KM=1,5
   11 AHALF = CUBE/2.0
      VOLUME = 8.0*AHALF**3
C**   AHALF IS HALF THE LENGTH OF A LITTLE CUBE EDGE   .
      ASQ = AHALF**2
C
      DO 350 I = IMIN,IMAX
      FI=I
      FKK=KK
      GO TO (864,865,866),NSFR
  864 JMAX = I
      GO TO 867
  865 FI=I
      JMAX=3.*FKK+0.5001-ABS(3.*FKK+0.5-FI)
      KFCC = 6*KK + 1
      GO TO 867
  866 JMAX=FKK+0.5001-ABS(FKK+0.5-FI)
  867 DO 350 J=1,JMAX
  868 DO 350 K = 1,J
      GO TO (345,870,345),NSFR
  870 IF(I+J+K-KFCC)345,345,350
  345 FJ=J
      FK=K
      Q(1)=(FI-0.5)*CUBE
```

```
      Q(2)=(FJ-0.5)*CUBE
      Q(3)=(FK-0.5)*CUBE
C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S). IS
C*     IF(JMAX.NE.J.AND.J.NE.K) 349,346
       IF((JMAX-J)*(J-K))349,346,349
  346  IF(K-JMAX)348,347,347
  347  U=1.0
       GO TO 19
  348  U = 3.0
       GO TO 19
  349  U = 6.0
   19  NS = NS + 1
       CALL FREQ(Q,GD1,GD2,GD3)
   31  IF(KG-1)34,34,29
   34  PRINT 105, NS,I,J,K,U,(Q(M),M=1,3),(V(M),M=1,NNN)
       PRINT 2000
       PRINT 2001, (FV(M,1), M = 1, NNN )
       PRINT 2002, (FV(M,2), M = 1, NNN )
       PRINT 2003, (FV(M,3), M = 1, NNN )
C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S). IS
C* 29  IF(KG.EQ.0.OR.KG.EQ.2) 35,370
   29  IF(KG*(KG-2))370,35,370
   35  CONTINUE
C
  370  CALL SWEEP(Q,GD1,GD2,GD3)
  350  CONTINUE
       PRINT 101
C
       SA = 0.0
C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S). IS
C*     IF(NCTA.GT.0.OR.NTAPE.GT.0.OR.IMIN.EQ.1) 47,68
       IF(NCTA)447,447,47
  447  IF(NTAPE)547,547,47
  547  IF(IMIN-1)68,47,68
   47  DO 56 I=1,LA
```

```
   56 SA = SA+CTA(I)                                                  170
      RA = 1.0E+08/SA                                                 171
      DO 57 J=1,LA                                                    172
      CTI(J)=CTI(J)*RA                                                172A
   57 CTA(J)=CTA(J)*RA                                                173
   68 PRINT 101
C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S), IS      175
C*    IF(NCTA.GT.0.AND.IMIN.GT.1) 63,66                               176
      IF(NCTA)66,66,163                                               177
  163 IF(IMIN-1)66,66,63                                              178
   63 CALL WRT (CTA,NDIMA,DVA,51,LA,1)
      PRINT 101
   66 IF(NTAPE)167,167,67                                             181
   67 CONTINUE
  167 CONTINUE                                                        183
      IF(IMIN-1)646,746,646                                           184
C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S), IS      185
C*646 IF(NCTA.GT.0.OR.NTAPE.GT.0) 46,746                              186
  646 IF(NCTA) 246,246,46                                             187
  246 IF(NTAPE) 746,746,46                                            188
   46 DO 146 J=1,LA
  146 CTA(J)=CTA(J)/RA                                                190
  746 PRINT 1112, KM, KK, NS, IMIN, IMAX
      PRINT 101
      KK = 3*KK                                                       193
      CUBE = CUBE/3.0                                                 194
      IMAX = (IMIN-1)*3                                               195
      GO TO (71,69,69,70,69),KM
   70 IMIN = 1                                                        197
      GO TO 69                                                        198
   71 IMIN = 4                                                        199
   69 CONTINUE                                                        200
C                                                                     201
  202 PRINT 1003
      PRINT 2120, (CTA(J),J=1, 50)
```

```
 201 DO 298 I=51,LA                                                     204
     CTI(I-50)=CTI(I)                                                   201A
 298 CTA(I-50)=3.0*CTA(I)
     NA = LA-50                                                         206
     NAA = NA + 1                                                       207
     DO 4000 J = NAA, LA                                                208
     CTI(J)=0.0                                                         208A
4000 CTA(J) = 0.0                                                       209
     IF(NCTA)6298,3298,3298                                             210
3298 PRINT 1002
     PRINT 9123, TITLE
     PRINT 7102, DVA
     PRINT 8123
     CALL WRT (CTA,NDIMA,DVA,1,NA,1)
     FRQ=-DVA/2.0                                                       212A
     DO 2020 I=1,NA                                                     212B
     FRQ=FRQ+DVA                                                        212C
2020 CTI(I)=3.0E-08*CTI(I)/FRQ                                          212D
     PRINT 1002                                                         212E
     CALL WRT(CTI,NDIMA,DVA,1,NA,2)
6298 CONTINUE
     IF (NPCH)  4299, 4301, 4299
4299 PUNCH 123, TITLE
     PUNCH 126, DVA, XM, NA, IDENT
     NCRD= NA/7 + 1
     K= 1
     DO 4300 I= 1, NCRD
     J= K + 6
     PUNCH 124, I, IDENT, (CTA(M), M= K,J)
4300 K= K+ 7
4301 CONTINUE
     IF (NPLOT) 4298,2298,4298
4298 PRINT 1002
     DO 4999 I=1,NA
4999 CTC(I)=CTA(I)
```

```
      CALL PLOT (0.,0.,0,100.,100.)                                     PLOTTERX
      CALL PLOT (80.0.,3)
      CALL FPLT (CTC,NDIMC,NA)
      CALL PLOT (0.,0.,2,100.,100.)
      CALL PLOT (30.,0.,2)
      CALL PLOT (0.,0.,0)
      DO 5011 I=1,NA                                                    216A
 5011 CTC(I)=CTI(I)*1.0E08
      CALL  FPLT(CTC,NDIMC,NA)
      CALL PLOT (0.,0.,-1)                                              PLOTTERX
 2298 PRINT 1002
      FRQ=-DVA/2.0
      FLAM=0.0
      DEGF=0.0                                                          234C
      DO 204 I=1,NA
      DEGF=DEGF+CTA(I)                                                  234E
      FRQ=FRQ+DVA
      FLAM=FLAM+2.0*CTI(I)/FRQ                                          234F
  204 CONTINUE
      PRINT 9126,DEGF                                                   234I
      PRINT 9127,FLAM
      TC=1.04*(1.0+FLAM)/(FLAM-FLE*(1.0+0.62*FLAM))
      TC=(THETA/1.45)*EXP(-TC)                                          234L
      PRINT 9128,TC                                                     234M
      END
      SUBROUTINE CONST                                                  235
C                                                                       236
C THIS SUBROUTINE SETS UP CONSTANTS, MULTIPLIES FORCE CONSTANTS         237
C BY CONVENIENT FACTORS, ETC., SO AS TO AVOID REPETITION IN             238
C SUBROUTINE FLEM .                                                     239
C                                                                       240
      DIMENSION PX(80), AMAS(12)                                        241
      COMMON/X2/ANN
      COMMON/X3/PI,CPT,PX,U,SC,NSFR,AMAS,DO
      COMMON/X7/N
```

```
C
      HH=1.66043
      PI=3.14159265
      SC=39.4784176*HH
  307 ANN = 0.5/(DQ*SC)
C  ANN AND SC ARE CHANGED FURTHER DOWN FOR FCC AND BCC .
C
      GO TO (51,52,53),NSER
C
C  SIMPLE CUBIC   (CESIUM CHLORIDE STRUCTURE)
   51 CPT=8.0*(PX(1)+PX(13)+2.0*PX(14))
  306 AMAS(1)=1.0/SQRT(AMAS(1))
      AMAS(2)=1.0/SQRT(AMAS(1))
      AMAS(3)=1.0/SQRT(AMAS(1))
      AMAS(4)=1.0/SQRT(AMAS(4))
      AMAS(5)=1.0/SQRT(AMAS(4))
      AMAS(6)=1.0/SQRT(AMAS(4))
C  IN THE CS-CL CASE, ARRAY AMAS CONTAINS 1/(SQRTS. OF MASSES) -
C  THESE ARE TAKEN INTO ACCOUNT BY SUBROUTINE ELEM .
      RETURN
C
C  FCC (MONATOMIC)
   52 CPT=2.0*(PX(4)+2.0*PX(5)+PX(25)+2.0*PX(26))
      ANN = ANN/AMAS(1)
      SC = SC*AMAS(1)
      DO 1 I = 1,3
    1 PX(I)=4.0*PX(I)
      PX(4)=2.0*PX(4)
      PX(5)=2.0*PX(5)
      DO 2 I=6,9
    2 PX(I)=8.0*PX(I)
      DO 3 I=10,16
    3 PX(I)=4.0*PX(I)
      DO 4 I=17,24
    4 PX(I)=8.0*PX(I)
```

```
      PX(25)=2.0*PX(25)
      PX(26)=2.0*PX(26)
      DO 1001  I=27,29
 1001 PX(I)=4.0*PX(I)
      DO 1002  I=30,33
 1002 PX(I)=8.0*PX(I)
      DO 1003  I=34,37
 1003 PX(I)=4.0*PX(I)
      DO 1004  I=38,41
 1004 PX(I)=8.0*PX(I)
      DO 1005 I=42,51
 1005 PX(I)=8.0*PX(I)
      DO 1006 I=52,55
 1006 PX(I)=4.0*PX(I)
      DO 1007 I=56,61
 1007 PX(I)=8.0*PX(I)
      DO 1008 I=62,64
 1008 PX(I)=4.0*PX(I)
      DO 1009 I=65,68
 1009 PX(I)=8.0*PX(I)
      DO 1010 I=69,72
 1010 PX(I)=4.0*PX(I)
      DO 1011 I=73,76
 1011 PX(I)=8.0*PX(I)
      PX(77)=2.0*PX(77)
      PX(78)=2.0*PX(78)
      RETURN
C
C BCC (MONATOMIC)
   53 CPT=2.0*(PX(3)+2.0*(PX(4)+PX(6)+2.0*(PX(1)
     1+PX(5)+PX(8)+PX(12)+2.0*PX(9))))+2.0*(PX(14)
     2+2.0*(PX(15)+2.0*(PX(16)+PX(20)+PX(21)+PX(22)
     3+2.0*PX(17))))
      ANN = ANN/AMAS(1)
      SC = SC*AMAS(1)
```

```
   90 RETURN
      END
      SUBROUTINE FREQ(Q,GD1,GD2,GD3)
C
      DIMENSION Q(3),F(12),A(12,12)
      DIMENSION EV(12,12),AA(12,12),DA(12,12),V(12),W(12),PX(80),QL(3)
      DIMENSION GD1(12),GD2(12),GD3(12),VL(12)
      DIMENSION AMAS (12)
      DIMENSION  BOG (12, 12)
      COMMON/X2/ANN
      COMMON/X3/PT,CPT,PX,U,SC,NSFR,AMAS,DQ
      COMMON/X4/EV,V
      COMMON/X7/N
      IF(Q(1).NE.Q(3)) GO TO 90
      IF(Q(1).NE.Q(2)) GO TO 90
      CALL ELEM(Q,A)
      V(1)=SQRT((A(1,1)+2.0*A(1,2))/SC)
      V(2)=SQRT((A(1,1)-A(1,2))/SC)
      V(3)=V(2)
      QL(1)=Q(1)+DQ
      QL(2)=QL(1)
      QL(3)=QL(1)
      CALL ELEM(QL,AA)
      VL(1)=SQRT((AA(1,1)+2.0*AA(1,2))/SC)
      VL(2)=SQRT((AA(1,1)-AA(1,2))/SC)
      VL(3)=VL(2)
      DO 731 I=1,3
      GD1(I)=(VL(I)-V(I))/DQ/3.
      GD2(I)=GD1(I)
  731 GD3(I)=GD1(I)
      RETURN
C
   90 FAC=0.0
      IF(U-1.0)10,1004,10
 1004 D10=1.0E-4
```

```
      D2Q=-1.0E-4                                                       303
      D3Q=1.0E-4                                                        304C
      Q(1)=Q(1)+D1Q                                                     305
      Q(2)=Q(2)+D2Q                                                     306
      Q(3)=Q(3)+D3Q                                                     307
      FAC=1.0                                                           308
   10 CALLELEM(Q,A)                                                     309
      DO 12 I=1,N                                                       310
      DO 12 J=1,N                                                       311
   12 EV(I, J)=A(I,J)
   15 CALL EIGEN (EV,E,3,1,12,BOG)
      DO 16 I=1,N                                                       314
   16 V(I)=SQRT(E(I)/SC)
   17 QL(1)=Q(1)+DQ                                                     316
      QL(2) = Q(2)                                                      317
      QL(3) = Q(3)                                                      318
      CALL ELEM(QL,AA)                                                  319
      DO 19 I=1,N                                                       320
      DO 19 J=1,I                                                       321
      DA(I,J)=AA(I,J)-A(I,J)
   19 DA(J,I)=AA(I,J)-A(I,J)
   22 CALL GRAD(DA,GD1)                                                 323
      IF(Q(1)-Q(2))24,23,24                                             324
   24 QL(1) = Q(1)                                                      325
      QL(2) = Q(2) + DQ                                                 326
      QL(3) = Q(3)                                                      327
      CALL ELEM(QL,AA)                                                  328
      DO 29 I=1,N                                                       329
      DO 29 J=1,I                                                       330
      DA(J,I)=AA(I,J)-A(I,J)
   29 DA(I,J)=DA(J,I)
   32 CALL GRAD(DA,GD2)                                                 332
      IF(Q(2)-Q(3))26,25,26                                             333
   23 DO 33 J=1,N                                                       334
   33 GD2(J)=GD1(J)                                                     335
```

```
 26 QL(1) = Q(1)
    QL(2) = Q(2)
    QL(3) = Q(3) + DQ
    CALL ELEM(QL,AA)
    Q(1)=Q(1)-FAC*D1Q
    Q(2)=Q(2)-FAC*D2Q
    Q(3)=Q(3)-FAC*D3Q
    DO 34 I=1,N
    DO 34 J=1,I
    DA(J,I)=AA(I,J)-A(I,J)
 34 DA(I,J)=DA(J,I)
 37 CALL GRAD(DA,GD3)
    DO 370 J=1,N
370 V(J)=V(J)-FAC*(GD1(J)*D1Q+GD2(J)*D2Q+GD3(J)*D3Q)
    RETURN
 25 DO 40 J=1,N
 40 GD3(J)=GD2(J)
 38 RETURN
    END
    SUBROUTINE ELEM(Q,A)
C
    DIMENSION A(12,12),Q(3),C(12,3),S(12,3),PX(80)
    DIMENSION AMAS(12)
    DIMENSION FV(12,12), V(12)
    COMMON/X3/PI,CPI,PX,U,SC,NSEB,AMAS,DQ
    COMMON/X4/FV,V
    COMMON/X7/N
C
    GO TO (1,2,3),NSEB
C
C  SIMPLE CUBIC (CESIUM CHLORIDE STRUCTURE)
C
  1 DO 510 I = 1,3
    S(1,I)=SIN(PI*Q(I))
    C(1,I)=COS(PI*Q(I))
    S(2,I)=2.0*S(1,I)*C(1,I)
```

```
      C(2,I)=1.0-2.0*S(1,I)**2
      S(3,I)=S(2,I)*C(1,I)+S(1,I)*C(2,I)
  510 C(3,I)=C(2,I)*C(1,I)-S(1,I)*S(2,I)
      DO 526 I = 1,3
  517 IF(I-3)512,511,512
  511 J = 1
      GO TO 513
  512 J = I+1
  513 IF(I-1)515,514,515
  514 K=3
      GO TO 516
  515 K = I-1
  5160 A(I,I)=CPT+2.0*(PX(3)*(1.0-C(2,I))+PX(5)*(2.0-C(2,J)-C(2,K))
     A  +2.0*(PX(7)*(2.0-C(2,I)*(C(2,J)+C(2,K)))+PX(9 )*(1.0-C(2,J)
     B   *C(2,K))))
     0A(I+3,I+3)=CPT+2.0*(PX(4)*(1.0-C(2,I))+PX(6)*(2.0-C(2,J)-C(2,K))
     A  +2.0*(PX(8)*(2.0-C(2,I)*(C(2,J)+C(2,K)))+PX(10)*(1.0-C(2,J)
     B   *C(2,K))))
     0            A(I+3,I)=-8.0*(C(1,J)*C(1,K)*(PX(1)*C(1,I)+PX(13)*
     A   C(3,I)))
       A(I,I+3)=A(I+3,I)
                A( J,I)=4.0*PX(11)*S(2,I)*S(2,J)
      A(I,J)=A( J,I)
                  A(J+3,I+3)=4.0*PX(12)*S(2,I)*S(2,J)
      A(I+3,J+3)=A(J+3,I+3)
     0                           A(J+3,I)=8.0*(S(1,I)*S(1,J)*(C(1,K)*
     A   PX(2)+PX(15)*C(3,K))+PX(16)*C(1,K)*(S(3,I)*S(1,J)+S(1,I)*
     B   S(3,J)))
                      A(J,I+3)=A(J+3,I)
                 A(I+3,J)=A(J,I+3)
       A(I, J+3)=A(I+3, J)
  526 CONTINUE
      DO 527 I = 1,N
      DO 527 J=1,N
  527 A(I,J) = A(I,J)*AMAS(I)*AMAS(J)
```

```
  518 RETURN                                                            400
C                                                                       401
C  FCC                                                                  402
C                                                                       403
    2 DO 125 I = 1,3                                                    404
      CON1=PI*Q(I)                                                      405
      S(1,I)=SIN(CON1)
      C(1,I)=COS(CON1)
      S(2,I)=2.0*S(1,I)*C(1,I)                                          408
      C(2,I)=1.0-2.0*S(1,I)**2                                          409
      S(3,I)=S(2,I)*C(1,I)+S(1,I)*C(2,I)                                410
      C(3,I)=C(2,I)*C(1,I)-S(1,I)*S(2,I)                                411
      S(4,I)=2.0*S(2,I)*C(2,I)                                          412
      C(4,I)=1.0-2.0*S(2,I)**2
      S(5,I)=S(3,I)*C(2,I) + C(3,I)*S(2,I)
      C(5,I)=C(3,I)*C(2,I) - S(3,I)*S(2,I)
      S(6,I)=2.*S(3,I)*C(3,I)
  125 C(6,I)=1.0-2.0*S(3,I)**2
      DO 126 I = 1,N                                                    414
  117 IF(I-3)112,111,112                                                415
  111 J = 1                                                             416
      GO TO 113                                                         417
  112 J = I+1                                                           418
  113 IF(I-1)115,114,115                                                419
  114 K=3                                                               420
      GO TO 116                                                         421
  115 K = I - 1                                                         422
  1160 A(I,I)=CPT+     PX(1)*(2.0-C(1,I)*(C(1,J)+C(1,K)))               423
     1   +  PX(2)*(1.0-C(1,J)*C(1,K))-     PX(4)*C(2,I)                 424
     2-     PX(5)*(C(2,J)+C(2,K))+     PX(6)*(1.0-C(2,I)*C(1,J)*        425
     3C(1,K))+     PX(7)*(2.0-C(1,I)*(C(2,J)*C(1,K)+C(1,J)*             426
     4C(2,K)))+     PX(10)*(2.0-C(2,I)*(C(2,J)+C(2,K)))                 427
     5+     PX(11)*(1.0-C(2,J)*C(2,K))                                  428
     6+     PX(13)*(2.0-C(3,I)*(C(1,J)+C(1,K)))                         429
     7+     PX(14)*(2.0-C(1,I)*(C(3,J)+C(3,K)))                         430
```

```
8+     PX(15)*(2.0-C(3,J)*C(1,K)-C(3,K)*C(1,J))                              431
9+     PX(17)*(1.0-C(2,I)*C(2,J)*C(2,K))                                     432
0  A0 = PX(19)*(2.0-C(3,I)*(C(2,J)*C(1,K)+C(1,J)*                          433
1C(2,K)))+                                                                  434
2    PX(20)*(2.0-C(2,I)*(C(1,J)*C(3,K)+C(3,J)*C(1,K)))                      435
3+     PX(21)*(2.0-C(1,I)*(C(3,J)*C(2,K)+C(2,J)*                            436
4C(3,K)))-    PX(26)*(C(4,J)+C(4,K))-    PX(25)*                           437
5C(4,I)                                                                     438
 A0D=PX(27)*(2.0-C(3,I)*(C(3,J)+C(3,K)))
1  +  PX(28)*(1.0-C(3,J)*C(3,K))
2  +PX(30)*  (1.0-C(4,I)*C(1,J)*C(1,K))
3  +  PX(31)*  (2.0-C(1,I)*  (C(1,J)*C(4,K)  + C(4,J)*C(1,K)))
4  +PX(34)  *  (2.0- C(4,I)  *  (C(2,J)  + C(2,K)))
5 + PX(35)  *  (2.0  - C(2,I)  *  (C(4,K)  + C(4,J)))
6  + PX(36)  *  (2.0  - C(4,J)  *  C(2,K)  -C(4,K)*C(2,J))
7  + PX(38)  *  (2.0  - C(3,I)  *  (C(3,J)*C(2,K)  + C(2,J)*C(3,K)))
8  + PX(39)  *  (1.0  - C(2,I)*C(3,J)*C(3,K))
 A(I,I)  =A(I,I)  +A0  +A0D
 A0D2= PX(42)*(1.0  - C(4,I)*C(2,J)*C(2,K))
1 + PX(43)*(2.0  - C(2,I)*(C(2,J)*C(4,K)  + C(4,J)*C(2,K)))
2 + PX(46)*(2.0-C(4,I)*(C(3,J)*C(1,K)  + C(1,J)*C(3,K)))
3 + PX(47)*(2.0-C(3,I)*(C(4,J)*C(1,K)  + C(1,J)*C(4,K)))
4 + PX(48)*(2.0-C(1,I)*(C(4,J)*C(3,K)  + C(3,J)*C(4,K)))
5  + PX(52)*(2.0-C(5,I)*(C(1,J)+C(1,K)))
6 + PX(53)*(2.0-C(1,I)*(C(5,J)  + C(5,K)))
7 + PX(54)*(2.0-C(5,J)*C(1,K)-C(1,J)*C(5,K))
8 + PX(56)*(2.0-C(5,I)*(C(2,J)*C(1,K)  + C(1,J)*C(2,K)))
9 + PX(57)*(2.0-C(2,I)*(C(5,J)*C(1,K)  + C(1,J)*C(5,K)))
1 + PX(58)*(2.0-C(1,I)*(C(5,J)*C(2,K)  + C(2,J)*C(5,K)))
 A0D3= PX(62)*(2.0-C(4,I)*(C(4,J)  + C(4,K)))
1 + PX(63)*(1.0-C(4,J)*C(4,K))
2 + PX(65)*(1.0-C(4,I)*C(3,J)*C(3,K))
3 + PX(66)*(2.0-C(3,I)*(C(3,J)*C(4,K)  + C(3,K)*C(4,J)))
4 + PX(69)*(2.0-C(5,I)*(C(3,J)  + C(3,K)))
5 + PX(70)*(2.0-C(3,I)*(C(5,J)  + C(5,K)))
```

```
6 + PX(71)*(2.0-C(3,J)*C(5,K) - C(3,K)*C(5,J))
7 + PX(73)*(2.0-C(4,I)*(C(4, J)*C(2,K) + C(4,K)*C(2,J)))
8 + PX(74)*(1.0-C(2,I)*C(4,J)*C(4,K))
9 + PX(77)*(1.0-C(6,I)) + PX(78)*(2.0-C(6,J)-C(6,K))
 A(I,I)=A(I,I) + A0D2 + A0D3
0          A(J,I)=     PX(3)*S(1,I)*S(1,J)+     PX(9)                       440
1*C(1,K)*(S(2,I)*S(1,J)+S(1,I)*S(2,J))+                                     441
2     PX(8)*S(1,I)*S(1,J)*C(2,K)+     PX(12)*S(2,I)*                        442
3S(2,J)+     PX(16)*(S(3,I)*S(1,J)+S(1,I)*S(3,J))+                          443
4     PX(18)*S(2,I)*S(2,J)*C(2,K)+                                          444
5     PX(24)*C(1,K)*(S(3,I)*S(2,J)+S(2,I)*                                  445
6S(3,J))+     PX(23)*C(2,K)*(S(1,I)*S(3,J)+S(3,I)*                          446
7S(1,J))+     PX(22)*C(3,K)*(S(1,I)*S(2, J)+S(2,I)*                         447
8S(1,J))                                                                    448
 A00=PX(29) *S(3,I) * S(3,J)
1  + PX(32) * C(4,K) *S(1,I) * S(1,J)
2 + PX(33) * C(1,K) * (S(1,I)*S(4,J) + S(4,I)*S(1,J))
3  + PX(37) * (S(4,I)*S(2,J) + S(2,I)*S(4,J))
4  + PX(40) * C(3,K) * (S(2,I)*S(3,J) + S(3,I)*S(2,J))
5  + PX(41) * C(2,K) * S(3,I) * S(3,J)
 A(J,I)=A(J,I) + A00
 A002= PX(44)*C(4,K)*S(2,I)*S(2,J)
1 + PX(45)*C(2,K)*(S(2,I)*S(4,J) + S(4,I)*S(2,J))
2 + PX(49)*C(4,K)*(S(3,I)*S(1,J) + S(1,I)*S(3,J))
3 + PX(50)*C(3,K)*(S(4,I)*S(1,J) + S(4,J)*S(1,I))
4 + PX(51)*C(1,K)*(S(4,I)*S(3,J) + S(3,I)*S(4,J))
5 + PX(55)*(S(5,I)*S(1,J) + S(1,I)*S(5,J))
6 + PX(59)*C(5,K)*(S(2,I)*S(1,J) + S(1,I)*S(2,J))
7 + PX(60)*C(2,K)*(S(5,I)*S(1,J) + S(1,I)*S(5,J))
8 + PX(61)*C(1,K)*(S(5,I)*S(2,J) + S(2,I)*S(5,J))
 A003= PX(64)*S(4,I)*S(4,J)
1 + PX(67)*C(4,K)*S(3,I)*S(3,J)
2 + PX(68)*C(3,K)*(S(4,I)*S(3,J) + S(3,I)*S(4,J))
3 + PX(72)*(S(5,I)*S(3,J) + S(3,I)*S(5,J))
4 + PX(75)*C(4,K)*(S(4,I)*S(2,J) + S(2,I)*S(4,J))
```

```
     5 + PX(76)*C(2,K)*S(4,I)*S(4,J)
       A(J,I)=A(J,I) + A002 + A003
        A(I,J)=A(J,I)
  126 CONTINUE
  118 RETURN
C
C  BCC
    3 DO 10 I = 1,3
      S(1,I)=SIN(PI*Q(I))
      C(1,I)=COS(PI*Q(I))
      S(2,I)=2.0*S(1,I)*C(1,I)
      C(2,I)=1.0-2.0*S(1,I)**2
      S(3,I)=S(2,I)*C(1,I)+S(1,I)*C(2,I)
      C(3,I)=C(2,I)*C(1,I)-S(1,I)*S(2,I)
      S(4,I)=2.0*S(2,I)*C(2,I)
   10 C(4,I)=1.0-2.0*S(2,I)**2
      DO 26 I=1,3
   17 IF(I-3)12,11,12
   11 J=1
      GO TO 13
   12 J=I+1
   13 IF(I-1)15,14,15
   14 K=3
      GO TO 16
   15 K=I-1
   160 A(I,I)=CPT-8.0*((PX(1)*C(1,I)+PX(8)*C(3,I))*
     1C(1,J)*C(1,K)+PX(12)*C(2,I)*C(2,J)*C(2,K)+
     2PX(9)*C(1,I)*(C(3,J)*C(1,K)+C(1,J)*C(3,K)))
     3-4.0*(PX(5)*C(2,I)*(C(2,J)+C(2,K))+PX(6)*C(2,J)*
     4C(2,K))-2.0*(PX(3)*C(2,I)+PX(4)*(C(2,J)+C(2,K)))
     5-8.0*(PX(16)*C(1,I)*C(3,J)*C(3,K)+
     6PX(17)*C(3,I)*(C(1,J)*C(3,K)+C(3,J)*C(1,K)))
     7-2.0*(PX(14)*C(4,I)+(PX(15)+2.0*PX(21)*C(2,I))*
     8(C(4,J)+C(4,K))+2.0*(PX(20)*C(4,I)*(C(2,J)+C(2,K))
     9+PX(22)*(C(4,J)*C(2,K)+C(2,J)*C(4,K))))
```

```
      0   A(J•I)=4.0*(PX(7)+2.0*PX(13)*C(2•K))                                    481
      1*S(2•I)*S(2•J)+4.0*PX(23)*(S(4•I)*S(2• J)+                                  482
      2S(2•I)*S(4•J))+8.0*(S(1•I)*S(1•J)*(PX(2)*                                   483
      3C(1•K)+PX(10)*C(3•K))+(PX(11)*C(1•K)+PX(18)                                 484C
      4*C(3•K))*(S(3•I)*S(1•J)+S(1•I)*S(3•J))+PX(19)                               485C
      5*S(3•I)*S(3•J)*C(1•K))                                                      486
       A(I•J)=A(J•I)
   26  CONTINUE                                                                    487
   18  RETURN                                                                      488
       END                                                                         489
       SUBROUTINE GRAD(A•G)                                                        556
C                                                                                  557
       DIMENSION FV(12•12)•A(12•12)•G(12)•P(12•12)•V(12)                           558
       COMMON/X2/ANN
       COMMON/X4/FV•V
       COMMON/X7/N
       DO10I=1•N                                                                   562
       Y=0.0                                                                       563
       DO11J=1•N                                                                   564
       X=0.0                                                                       565
       DO12K=1•N                                                                   566
   12  X=X+FV(K•I)*A(K•J)                                                          567
   11  P(I•J)=X                                                                    568
       DO13K=1•N                                                                   569
   13  Y=Y+P(I•K)*FV(K•I)                                                          570
   10  G(I) = Y*ANN/V(I)                                                           571
       RETURN                                                                      572
       END                                                                         573
       SUBROUTINE SWEEP(Q•GD1•GD2•GD3)                                             574
C                                                                                  575
       COMMON/X3/PI•CPT•PX•U•SC•NSFB•AMAS•DQ
       COMMON/X4/FV•V
       COMMON/X5/LA•CTA•DVA•AHALF•VOLUME•ASQ•NPRINT,XM
       COMMON/X6/KM•KQ•IZ•JZ•KZ
       COMMON/X7/NNN
```

```
      COMMON/X8/ALP,EKE,RHO,EP,Z,POTEN,CTI,AMASS,OMEGA                  580A
      DIMENSION CTA(1500),AL(3),V(12),GD1(12),GD2(12),GD3(12)           581
      DIMENSION PX(80),Q(3)                                             582
      DIMENSION AMAS(12)                                                583
      DIMENSION EV(12,12)                                               584
      DIMENSION CTI(1500),UM(3),POTEN(7)                                584A
 1000 FORMAT(5X, 7F11.6, 2F15.5, I6)                                    586
 1002 FORMAT(26H V(L).GT.MAX FREQ  V(L) =  ,F15.6/ 1HK)                 587
      EPC=0.0                                                           588A
      DO 14 I=1,8
      DO 13 J=1,8
      DO 12 K=1,8
      LCEN=I+J+K
      IF (LCEN.EQ. 4) GO TO 12
      IF (LCEN.EQ. 6) GO TO 12
      IF (LCEN.EQ. 8) GO TO 12
      IF (LCEN.EQ.10) GO TO 12
      IF (LCEN.EQ.12) GO TO 12
      IF (LCEN.EQ.14) GO TO 12
      IF (LCEN.EQ.16) GO TO 12
      UM(1)=(1.0E-29+I-1.0)/2.0
      UM(2)=(1.0E-29+J-1.0)/2.0
      UM(3)=(1.0E-29+K-1.0)/2.0
      UMK=(UM(1)+Q(1))**2+(UM(2)+Q(2))**2+(UM(3)+Q(3))**2               588H
      UMK=SQRT(UMK)                                                     588I
      TEST=2.0*EKE-(6.2831853/ALP)*UMK                                  588J
      IF(TEST) 12,10,10                                                 588K
   10 CONTINUE                                                          588L
      UMK=6.2831853/ALP*UMK
      CALL EPH (UMK,AMASS,OMEGA,Z,RHO,EKE,POTEN,EP,ALPHA)               588M
      EPC=EPC+ALPHA                                                     588N
   12 CONTINUE                                                          588P
   13 CONTINUE                                                          588Q
   14 CONTINUE                                                          588R
      DO 20 L = 1,NNN                                                   589
```

```
      IF(V(L)-XM)21,19,19                                          590C
   19 PRINT 1002, V(L)
      GO TO 20                                                     592
   21 GRD=SQRT(GD1(L)**2+GD2(L)**2+GD3(L)**2)
      DFLW=DVA/GRD                                                 594
      AL(1)=ABS(GD1(L))/GRD
      AL(2)=ABS(GD2(L))/GRD
      AL(3)=ABS(GD3(L))/GRD
      ALMN=1.0/(AL(1)*AL(2)*AL(3))                                 598
      IF(AL(1) - AL(2)) 521,522,522                                599C
  521 AP=AL(1)                                                     600
      AL(1)=AL(2)                                                  601
      AL(2)=AP                                                     602
  522 IF(AL(2)-AL(3)) 523,527,527                                  603C
  523 IF(AL(3)-AL(1)) 524,525,525                                  604C
C                                                                  605
  524 AP=AL(2)                                                     606
      AL(2)=AL(3)                                                  607
      AL(3)=AP                                                     608
      GO TO 527                                                    609
  525 AP=AL(3)                                                     610
      AL(3)=AL(2)                                                  611
      AL(2)=AL(1)                                                  612
      AL(1)=AP                                                     613
  527 CONTINUE                                                     614
      W1=(-AL(1)+AL(2)+AL(3))*AHALF                                615
      W2=(AL(1)-AL(2)+AL(3))*AHALF                                 616
      W3=(AL(1)+AL(2)-AL(3))*AHALF                                 617
      W4=(AL(1)+AL(2)+AL(3))*AHALF                                 618
C                                                                  619
C   CONSTANTS NEEDED                                               620
      ULMN = U*ALMN                                                621
      CON = 0.5*ULMN                                               622
      WSQ = W1**2                                                  623
      AL23 = 4.0*AL(2)*AL(3)*ASQ                                   624
```

```
      B3 = CON*W4
      A3 = B3*W4
      C3 = ULMN/6.0
      B42 = ULMN*AHALF*AL(3)
      A42 = 2.0*B42*AHALF*(AL(1)+AL(2))
      A5 = CON*(2.0*AL23 - WSQ)
      B5 = CON*W1
      C5 = -C3
      A6 = ULMN*(AL23 - WSQ)
      A41=4.0*U*ASQ/AL(1)
      SUM = 0.0
C
      DO 900 JJJ = 1.7
      GO TO (751.752.753.754.755.756.757).JJJ
  751 A = A3
      B = B3
      C = C3
      WN = -W4
      WX = -W3
      FMAX = V(L) + WN*GRD
      NN2 = FMAX/DVA + 1.0
      AN2 = NN2 - 1
      N2 = NN2 + 50
      NMIN = N2
      BW = (FMAX - AN2*DVA)/GRD
      GO TO 770
C
  752 A = A42
      B = B42
      C = 0.0
      WX = -W2
      GO TO 770
C
  753 A = A5
      B = B5
```

```
      C = C5
      WX=-ABS(W1)
      GO TO 770
C
  754 IF(W1) 4754.900.6754
 4754 A = A41
      B = 0.0
      C = 0.0
      WX = -W1
      GO TO 770
C
 6754 A = A6
      B = 0.0
      C = -ULMN/3.0
      WX = W1
      GO TO 770
C
  755 A = A5
      B = -B5
      C = C5
      WX = W2
      GO TO 770
C
  756 A = A42
      B = -B42
      C = 0.0
      WX = W3
      GO TO 770
C
  757 A = A3
      B = -B3
      C = C3
      WX = W4
C
  770 FMIN = FMAX
```

```
      FMAX = V(L) + WX*GRD
      N1 = N2
      NN2 = FMAX/DVA + 1.0
      AN2 = NN2 - 1
      N2 = NN2+50
      AW = DELW - BW
      BW = (FMAX - AN2*DVA)/GRD
      IF(N2-N1) 850,850,780
  780 NFRST = N1 + 1
      NLAST = N2 - 1
      W = WN + AW
C
      DELN = AW*(A + B*(WN+W) + C*(WN**2+WN*W+W**2))
      CTA(N1) = DELN + CTA(N1)
      CTT(N1)=EPC*DELN+CTT(N1)
      SUM = SUM+DELN
      IF(NLAST.LT.NFRST) GO TO 825
C
      DO 800 KN = NFRST,NLAST
      WW = W + DELW
      DELN = DELW*(A + B*(W+WW) + C*(W**2+W*WW+WW**2))
      CTT(KN)=EPC*DELN+CTT(KN)
      CTA(KN) = DELN + CTA(KN)
      SUM = SUM + DELN
  800 W = W + DELW
C
  825 WW = W + BW
      DELN = BW*(A + B*(W+WW) + C*(W**2+W*WW+WW**2))
      CTT(N2)=EPC*DELN+CTT(N2)
      CTA(N2) = DELN + CTA(N2)
      SUM = SUM + DELN
      W = WW
      GO TO 900
C
  850 CW = WX - WN
```

```
      DELN = CW*(A + B*(WN+WX) + C*(WN**2+WN*WX+WX**2))                 727
      CTT(N1)=EPC*DELN+CTT(N1)                                          727A
      CTA(N1) = DELN + CTA(N1)                                          728
      SUM = SUM + DELN                                                  729
  900 WN = WX                                                           730
C                                                                       731
      GO TO (20,30),NPRINT                                              732
   30 SUM = SUM/U                                                       733
      NDEL = N2 - NMIN + 1                                              734
 7654 DIFF = VOLUME - SUM                                               735
      PRINT 1000, V(I), GRD,AL(1),AL(2),AL(3),DELW,W1,VOLUME,DIFF,NDEL
C  THE VOLUME PRINTED HERE IS THE CORRECT VALUE . DIFF=CORRECT-SUMMED   737
C                                                                       738
   20 CONTINUE                                                          739
   26 CONTINUE
      RETURN                                                            740
      END                                                               741
      SUBROUTINE WRT (ARRAY,NDIM,DELF,NA,NB,NFMT)
C                                                                       743
      DIMENSION ARRAY(NDIM)                                             744
  101 FORMAT(1X,F10.5,7X,10F11.0)                                       745
  102 FORMAT(1X,F10.5,7X,10F10.3)                                       746
C                                                                       747
      NLINES = (NB-NA+9)/10                                             748
      N2 = NA-1                                                         749
      FINCR=10.*DELF                                                    750
      FRQ = -FINCR                                                      751
      DO 5 J=1,NLINES                                                   752
      N1=N2+1                                                           753
      N2=N1+9                                                           754
      FRQ=FRQ+FINCR                                                     755
      GO TO (1,2),NFMT
    1 PRINT 101, FRQ, (ARRAY(K), K=N1, N2)
      GO TO 5                                                           758
    2 PRINT 102, FRQ, (ARRAY(K), K=N1, N2)
```

```
    5 CONTINUE                                                          760
      RETURN                                                            761
      END                                                               762
      SUBROUTINE EIGEN(A,VALU,N,M,IA,B)                                 IEI00001
C     F4 UCSD EIGEN                                                F 63 IEI00002
C                                                                       IEI00004
C                                                                       IEI00005
C     EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC MATRIX           IEI00003
      DIMENSION A(IA,1),B(IA,1),VALU(20),DIAG(20),SUPERD(19),           IEI00006
     X          Q(19), VALL(20), S(19), C(19), D(20), IND(20), U(20)    IEI00007
C                                                                       IEI00008
C     CALCULATE NORM OF MATRIX                                          IEI00009
C                                                                       IEI00010
    3 ANORM2=0.0                                                        IEI00011
    4 DO 6 I=1,N                                                        IEI00012
    5 DO 6 J=1,N                                                        IEI00013
    6 ANORM2=ANORM2+A(I, J)**2                                          IEI00014
    7 ANORM=SQRTF(ANORM2)                                               IEI00015
C                                                                       IEI00016
C     GENERATE IDENTITY MATRIX                                          IEI00017
C                                                                       IEI00018
    9 IF (M) 10, 45, 10                                                 IEI00019
   10 DO 40 I=1,N                                                       IEI00020
   12 DO 40 J=1,N                                                       IEI00021
   20 IF(I-J) 35, 25, 35                                                IEI00022
   25 B(I,J)=1.0                                                        IEI00023
   30 GO TO 40                                                          IEI00024
   35 B(I,J)=0.0                                                        IEI00025
   40 CONTINUE                                                          IEI00026
C                                                                       IEI00027
C     PERFORM ROTATIONS TO REDUCE MATRIX TO JACOBI FORM                 IEI00028
C                                                                       IEI00029
   45 IEXIT=1                                                           IEI00030
   50 NN=N-2                                                            IEI00031
   52 IF (NN) 890, 170, 55                                              IEI00032
```

```
   55 DO 160 I=1.NN                                                     IFI00033
   60 II=I+2                                                            IFI00034
   65 DO 160 J=II.N                                                     IFI00035
   70 T1=A(I.I+1)                                                       IFI00036
   75 T2=A(I.J)                                                         IFI00037
   80 GO TO 900                                                         IFI00038
   90 DO 105 K=I.N                                                      IFI00039
   95 T2=COS*A(K.I+1)+SIN*A(K.J)                                        IFI00040
  100 A(K.J)=COS*A(K. J)-SIN*A(K.I+1)                                   IFI00041
  105 A(K.I+1)=T2                                                       IFI00042
  110 DO 125 K=I.N                                                      IFI00043
  115 T2=COS*A(I+1.K)+SIN*A(J.K)                                        IFI00044
  120 A( J.K)=COS*A( J.K)-SIN*A(I+1.K)                                  IFI00045
  125 A(I+1.K)=T2                                                       IFI00046
  128 IF (M) 130. 160. 130                                              IFI00047
  130 DO 150 K=1.N                                                      IFI00048
  135 T2=COS*B(K.I+1)+SIN*B(K.J)                                        IFI00049
  140 B(K.J)=COS*B(K. J)-SIN*B(K.I+1)                                   IFI00050
  150 B(K.I+1)=T2                                                       IFI00051
  160 CONTINUE                                                          IFI00052
C                                                                       IFI00053
C     MOVE JACOBI FORM ELEMENTS AND INITIALIZE EIGENVALUE BOUNDS        IFI00054
C                                                                       IFI00055
  170 DO 200 I=1.N                                                      IFI00056
  180 DIAG(I)=A(I.I)                                                    IFI00057
  190 VALU(I)=ANORM                                                     IFI00058
  200 VALL(I)=-ANORM                                                    IFI00059
  210 DO 230 I=2.N                                                      IFI00060
  220 SUPERD(I-1)=A(I-1.I)                                              IFI00061
  230 Q(I-1)=(SUPERD(I-1))**2                                           IFI00062
C                                                                       IFI00063
C     DETERMINE SIGNS OF PRINCIPAL MINORS                               IFI00064
C                                                                       IFI00065
  235 TAU=0.0                                                           IFI00066
  240 I=1                                                               IFI00067
```

```
  260 MATCH=0                                                           IFI00068
  270 T2=0.0                                                            IFI00069
  275 T1=1.0                                                            IFI00070
  277 DO 450 J=1,N                                                      IFI00071
  280 P=DIAG(J)-TAU                                                     IFI00072
  290 IF(T2) 300, 330, 300                                              IFI00073
  300 IF(T1) 310, 370, 310                                              IFI00074
  310 T=P*T1-Q(J-1)*T2                                                  IFI00075
  320 GO TO 410                                                         IFI00076
  330 IF(T1) 335, 350, 350                                              IFI00077
  335 T1=-1.0                                                           IFI00078
  340 T=-P                                                              IFI00079
  345 GO TO 410                                                         IFI00080
  350 T1=1.0                                                            IFI00081
  355 T=P                                                               IFI00082
  360 GO TO 410                                                         IFI00083
  370 IF(Q(J-1)) 380, 350, 380                                          IFI00084
  380 IF(T2) 400, 390, 390                                              IFI00085
  390 T=-1.0                                                            IFI00086
  395 GO TO 410                                                         IFI00087
  400 T=1.0                                                             IFI00088
C                                                                       IFI00089
C     COUNT AGREEMENTS IN SIGN                                          IFI00090
C                                                                       IFI00091
  410 IF(T1) 425, 420, 420                                              IFI00092
  420 IF(T) 440, 430, 430                                               IFI00093
  425 IF(T) 430, 440, 440                                               IFI00094
  430 MATCH=MATCH+1                                                     IFI00095
  440 T2=T1                                                             IFI00096
  450 T1=T                                                              IFI00097
C                                                                       IFI00098
C     ESTABLISH TIGHTER BOUNDS ON EIGENVALUES                           IFI00099
C                                                                       IFI00100
  460 DO 530 K=1,N                                                      IFI00101
  465 IF (K-MATCH) 470, 470, 520                                        IFI00102
```

```
  470 IF(TAU-VALL(K)) 530, 530, 480                                      IFI00103
  480 VALL(K)=TAU                                                        IFI00104
  490 GO TO 530                                                          IFI00105
  520 IF(TAU-VALU(K)) 525, 530, 530                                      IFI00106
  525 VALU(K)=TAU                                                        IFI00107
  530 CONTINUE                                                           IFI00108
  540 IF(VALU(I)-VALL(I)-5.0E-8) 570, 570, 550                           IFI00109
  550 IF(VALU(I)) 560, 580, 560                                          IFI00110
  560 IF(ABSF(VALL(I)/VALU(I)-1.0)-5.0E-8) 570, 570, 580                 IFI00111
  570 I=I+1                                                              IFI00112
  575 IF(I-N) 540, 540, 590                                              IFI00113
  580 TAU=(VALL(I)+VALU(I))/2.0                                          IFI00114
  585 GO TO 260                                                          IFI00115
C                                                                        IFI00116
C       JACOBI EIGENVECTORS BY ROTATIONAL TRIANGULARIZATION              IFI00117
C                                                                        IFI00118
  590 IF (M) 593, 890, 593                                               IFI00119
  593 IEXIT=2                                                            IFI00120
  595 DO 610 I=1,N                                                       IFI00121
  600 DO 610 J=1,N                                                       IFI00122
  610 A(I,J)=0.0                                                         IFI00123
  615 DO 850 I=1,N                                                       IFI00124
  620 IF (I-1) 625, 625, 621                                             IFI00125
  621 IF (VALU(I-1)-VALU(I)-5.0E-7) 730, 730, 622                        IFI00126
  622 IF (VALU(I-1)) 623, 625, 623                                       IFI00127
  623 IF (ABSF(VALU(I)/VALU(I-1)-1.0)-5.0E-7) 730, 730, 625              IFI00128
  625 COS=1.0                                                            IFI00129
  628 SIN=0.0                                                            IFI00130
  630 DO 700 J=1,N                                                       IFI00131
  635 IF(J-1) 680, 680, 640                                              IFI00132
  640 GO TO 900                                                          IFI00133
  650 S(J-1)=SIN                                                         IFI00134
  660 C(J-1)=COS                                                         IFI00135
  670 D(J-1)=T1*COS+T2*SIN                                               IFI00136
  680 T1=(DIAG(J)-VALU(I))*COS-BETA*SIN                                  IFI00137
```

```
  690 T2=SUPERD(J)                                                        IFI00138
  700 BETA=SUPERD(J)*COS                                                  IFI00139
  710 D(N)=T1                                                             IFI00140
  720 DO 725 J=1,N                                                        IFI00141
  725 IND(J)=0                                                            IFI00142
  730 SMALLD=ANORM                                                        IFI00143
  735 DO 780 J=1,N                                                        IFI00144
  740 IF (IND(J)-1) 750, 780, 780                                         IFI00145
  750 IF (ABSF(SMALLD)-ABSF(D(J)))780, 780, 760                           IFI00146
  760 SMALLD=D(J)                                                         IFI00147
  770 NN=J                                                                IFI00148
  780 CONTINUE                                                            IFI00149
  790 IND(NN)=1                                                           IFI00150
  800 PRODS=1.0                                                           IFI00151
  805 IF (NN-1) 810, 850, 810                                             IFI00152
  810 DO 840 K=2,NN                                                       IFI00153
  820 II=NN+1-K                                                           IFI00154
  830 A(II+1,I)=C(II)*PRODS                                               IFI00155
  840 PRODS=-PRODS*S(II)                                                  IFI00156
  850 A(1,I)=PRODS                                                        IFI00157
C                                                                         IFI00158
C     FORM MATRIX PRODUCT OF ROTATION MATRIX WITH JACOBI VECTOR MATRIX    IFI00159
C                                                                         IFI00160
  855 DO 885 J=1,N                                                        IFI00161
  860 DO 865 K=1,N                                                        IFI00162
  865 U(K)=A(K,J)                                                         IFI00163
  870 DO 885 I=1,N                                                        IFI00164
  875 A(I,J)=0.0                                                          IFI00165
  880 DO 885 K=1,N                                                        IFI00166
  885 A(I,J)=B(I,K)*U(K)+A(I,J)                                           IFI00167
  890 RETURN                                                              IFI00168
C                                                                         IFI00169
C     CALCULATE SINE AND COSINE OF ANGLE OF ROTATION                      IFI00170
C                                                                         IFI00171
  900 IF (T2) 910, 940, 910                                               IFI00172
  910 T=SQRTF(T1**2+T2**2)                                                IFI00173
```

```
920 COS=T1/T                                                                 IFI00174
925 SIN=T2/T                                                                 IFI00175
930 GO TO (90,650), IFXIT                                                    IFI00176
940 GO TO (160,910), IFXIT                                                   IFI00177
950 END                                                                      IFI00178
    SUBROUTINE FPLT (C,NDIMC,N)
    DIMENSION C(NDIMC)                                                       PLOTTERX
100 FORMAT (////,10X,13HPLOT OF G(NU)   )                                    PLOTTERX
101 FORMAT (14H0VALUE OF TT =, F15.6)                                        PLOTTERX
102 FORMAT (49H0FREQUENCY PLOTTED ON X AXIS, 1 MARK = 0.1 V/VMAX )           PLOTTERX
103 FORMAT (48H0NORMALIZED DISTRIBUTION, ON Y AXIS 1 MARK = 0.2   )          PLOTTERX
    PRINT 100                                                                PLOTTERX
    TT=0.                                                                    PLOTTERX
    DO 1 I=1,N                                                               PLOTTERX
  1 TT=TT+C(I)                                                               PLOTTERX
    PRINT 101, TT                                                            PLOTTERX
    PRINT 102                                                                PLOTTERX
    PRINT 103                                                                PLOTTERX
    NO=N                                                                     PLOTTERX
  2 IF(C(NO)-1.) 3,4,4                                                       PLOTTERX
  3 NO=NO-1                                                                  PLOTTERX
    GO TO 2                                                                  PLOTTERX
  4 NO=NO+1                                                                  PLOTTERX
    MO=1
    ANO=NO
 41 ANO=ANO/10.0
    MO=MO*10
    IF (ANO-10.0) 43,43,41
 43 NO=ANO+1
    MO=MO*NO
    D=1.0/MO
    CMAX=0.0
    DO 52 I=1,MO
    IF (CMAX-C(I)) 51,51,52
 51 CMAX=C(I)
 52 CONTINUE
```

```
      KO=1
   53 CMAX=CMAX/10.0
      KO=KO*10
      IF (CMAX-10.0) 55,55,53
   55 MAX=INT(CMAX)+1
      HEIGHT=5.0/8.0
      WIDTH=8.0/5.0
      SYP=2000.0*HEIGHT
      SXP=1000.0*WIDTH
      XS=WIDTH*10.0/FLOAT(NO)
      YS=HEIGHT*16.0/FLOAT(MAX)
      CALL PLOT (0.,-60.,2)                                         PLOTTERX
      CALL PLOT (0.,0.,0)                                           PLOTTERX
      CALL PLOT (5.,10.,2)                                          PLOTTER
      CALL PLOT (0.,0.,0)                                           PLOTTERX
      X=0.                                                          PLOTTERX
      DO 6 I=1,NO
      X=X+XS                                                        PLOTTERX
      CALL PLOT (0.,X,1)                                            PLOTTERX
      CALL PLOT (0.1,X,1)                                           PLOTTERX
    6 CALL PLOT (0.,X,1)                                            PLOTTERX
      CALL PLOT (0.,0.,1)                                           PLOTTERX
      Y=0.                                                          PLOTTERX
      DO 7 I=1,MAX
      Y=Y+YS
      CALL PLOT (Y,0.,1)                                            PLOTTERX
      CALL PLOT (Y,0.1,1)                                           PLOTTERX
    7 CALL PLOT (Y,0.,1)                                            PLOTTERX
      CALL PLOT (0.,0.,1)                                           PLOTTERX
      DO 8 I=1,MO
      X=I*D                                                         PLOTTERX
      Y=8.0*C(I)/(10.0*FLOAT(KO)*FLOAT(MAX))
    8 CALL PLOT (Y,X,1,SYP,SXP)                                     PLOTTERX
      RETURN                                                        PLOTTERX
      END                                                           PLOTTERX
      SUBROUTINE EPH (Q,AMASS,OMEGA,Z,RHO,FKF,POTEN,FP,ALPHA)
      DIMENSION POTEN(7),FACT(7)
```

```
      COMPLEX SUM,COMP,CONG,G,GBAR
      FACT(1)=1.0 $ FACT(2)=1.0 $ FACT(3)=2.0 $ FACT(4)=6.0$FACT(5)=24.0
      FACT(6)=120.0 $ FACT(7)=720.0 $ PI=3.14159265 $ SUM=(0.0,0.0)
      ELCHG=4.80298E-10 $ HBAR=1.0545E-27 $ EMASS=9.1091E-28
      ELCHSQ=ELCHG**2 $ HBARSQ=HBAR**2
C     CALCULATE HARTREE SCREENING
      HARTRE=((4.0*FKF**2-Q**2)/(8.0*FKF*Q))*ALOG((2.0*FKF+Q)/
     1(2.0*FKF-Q))
      HARTRE=HARTRE+0.5
      HARTRE=((8.0*ELCHSQ*EMASS*FKF)/(HBARSQ*Q**2*PI))*HARTRE
C     CALCULATE EXCHANGE SCREENING
      EXCH=0.693147*RHO*8.0*PI*ELCHSQ/(Q*FKF)
C     FIND TOTAL SCREENING
      SCREEN=1.0+HARTRE-EXCH
C FIND BARE COUPLING TIMES SQRT OF THE QUANTITY,FREQ TIMES LATTICE POINTS
      DENOM=FP**2+Q**2
      COMP=(1.0,0.0)*FP+(0.0,1.0)*Q
      CONG=(1.0,0.0)*FP-(0.0,1.0)*Q
      DO 10 J=1,7
   10 SUM=FACT(J)*POTEN(J)*(COMP**J-CONG**J)/(DENOM**J)
      SUM=34.0*(0.0,1.0)*SUM/Q
      G=PI*(Z-68.0)/(2.0*Q)+68.0*ATAN2(Q,FP)/Q+SUM
      G=(4.0*PI*ELCHSQ*(0.0,1.0)/OMEGA)*SQRT(HBAR)/(SQRT(AMASS)*1.41421
     13562)*G
      GBAR=G/SCREEN
      GBAR=GBAR/1.414213562
      GBAR=CONJG(GBAR)*GBAR
      GREAL=REAL(GBAR)
      ALPHA=GREAL
C     INCLUDE FACTOR OF N(0)/(8*PI*FKF**2*Q)*(2*PI)**3
      ALPHA=ALPHA*RHO*PI**2/(Q*FKF**2)
      RETURN
      END
```

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36. Electrons distort a small region of the lattice about their position. It is this virtual phonon cloud which is felt by another electron that forms the attractive mechanism. Normal coulomb repulsion is, of course, still present.

37. The reason that $\bar{g}'$ is indicated instead of g' is that the screened electron-phonon coupling constant $\bar{g}$ will be sought self-consistently instead of the bare ion coupling g.

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```
920 COS=T1/T                                                            IFI00174
925 SIN=T2/T                                                            IFI00175
930 GO TO (90,650), IFXIT                                               IFI00176
940 GO TO (160,910), IFXIT                                              IFI00177
950 END                                                                 IFI00178
    SUBROUTINE EPLT (C,NDIMC,N)
    DIMENSION C(NDIMC)                                                  PLOTTERX
100 FORMAT (////,10X,13HPLOT OF G(NU)   )                               PLOTTERX
101 FORMAT (14H0VALUE OF TT =, F15.6)                                   PLOTTERX
102 FORMAT (49H0FREQUENCY PLOTTED ON X AXIS, 1 MARK = 0.1 V/VMAX )      PLOTTERX
103 FORMAT (48H0NORMALIZED DISTRIBUTION, ON Y AXIS 1 MARK = 0.2  )      PLOTTERX
    PRINT 100                                                           PLOTTERX
    TT=0.                                                               PLOTTERX
    DO 1 I=1,N                                                          PLOTTERX
  1 TT=TT+C(I)                                                          PLOTTERX
    PRINT 101, TT                                                       PLOTTERX
    PRINT 102                                                           PLOTTERX
    PRINT 103                                                           PLOTTERX
    NO=N                                                                PLOTTERX
  2 IF(C(NO)-1.) 3,4,4                                                  PLOTTERX
  3 NO=NO-1                                                             PLOTTERX
    GO TO 2                                                             PLOTTERX
  4 NO=NO+1                                                             PLOTTERX
    MO=1
    ANO=NO
 41 ANO=ANO/10.0
    MO=MO*10
    IF (ANO-10.0) 43,43,41
 43 NO=ANO+1
    MO=MO*NO
    D=1.0/MO
    CMAX=0.0
    DO 52 I=1,MO
    IF (CMAX-C(I)) 51,51,52
 51 CMAX=C(I)
 52 CONTINUE
```

```
      KO=1
   53 CMAX=CMAX/10.0
      KO=KO*10
      IF (CMAX-10.0) 55,55,53
   55 MAX=INT(CMAX)+1
      HEIGHT=5.0/8.0
      WIDTH=8.0/5.0
      SYP=2000.0*HEIGHT
      SXP=1000.0*WIDTH
      XS=WIDTH*10.0/FLOAT(NO)
      YS=HEIGHT*16.0/FLOAT(MAX)
      CALL PLOT (0.,-60.,2)                                             PLOTTERX
      CALL PLOT (0.,0.,0)                                               PLOTTERX
      CALL PLOT (5.,10.,2)                                              PLOTTER
      CALL PLOT (0.,0.,0)                                               PLOTTERX
      X=0.                                                              PLOTTERX
      DO 6 I=1,NO
      X=X+XS                                                            PLOTTERX
      CALL PLOT (0.,X,1)                                                PLOTTERX
      CALL PLOT (0.1,X,1)                                               PLOTTERX
    6 CALL PLOT (0.,X,1)                                                PLOTTERX
      CALL PLOT (0.,0.,1)                                               PLOTTERX
      Y=0.                                                              PLOTTERX
      DO 7 I=1,MAX
      Y=Y+YS
      CALL PLOT (Y,0.,1)                                                PLOTTERX
      CALL PLOT (Y,0.1,1)                                               PLOTTERX
    7 CALL PLOT (Y,0.,1)                                                PLOTTERX
      CALL PLOT (0.,0.,1)                                               PLOTTERX
      DO 8 I=1,MO
      X=I*D                                                             PLOTTERX
      Y=8.0*C(I)/(10.0*FLOAT(KO)*FLOAT(MAX))
    8 CALL PLOT (Y,X,1,SYP,SXP)                                         PLOTTERX
      RETURN                                                            PLOTTERX
      END                                                               PLOTTERX
      SUBROUTINE FPH (Q,AMASS,OMEGA,Z,RHO,FKF,POTEN,FP,ALPHA)
      DIMENSION POTEN(7),FACT(7)
```

```
      COMPLEX SUM,COMP,CONG,G,GBAR
      FACT(1)=1.0 $ FACT(2)=1.0 $ FACT(3)=2.0 $ FACT(4)=6.0$FACT(5)=24.0
      FACT(6)=120.0 $ FACT(7)=720.0 $ PI=3.14159265 $ SUM=(0.0,0.0)
      ELCHG=4.80298E-10 $ HBAR=1.0545E-27 $ EMASS=9.1091E-28
      ELCHSQ=ELCHG**2 $ HBARSQ=HBAR**2
C     CALCULATE HARTREE SCREENING
      HARTRE=((4.0*FKF**2-Q**2)/(8.0*FKF*Q))*ALOG((2.0*FKF+Q)/
     1(2.0*FKF-Q))
      HARTRE=HARTRE+0.5
      HARTRE=((8.0*ELCHSQ*EMASS*FKF)/(HBARSQ*Q**2*PI))*HARTRE
C     CALCULATE EXCHANGE SCREENING
      EXCH=0.693147*RHO*8.0*PI*ELCHSQ/(Q*FKF)
C     FIND TOTAL SCREENING
      SCREEN=1.0+HARTRE-EXCH
C FIND BARE COUPLING TIMES SQRT OF THE QUANTITY,FREQ TIMES LATTICE POINTS
      DENOM=FP**2+Q**2
      COMP=(1.0,0.0)*FP+(0.0,1.0)*Q
      CONG=(1.0,0.0)*FP-(0.0,1.0)*Q
      DO 10 J=1,7
   10 SUM=FACT(J)*POTEN(J)*(COMP**J-CONG**J)/(DENOM**J)
      SUM=34.0*(0.0,1.0)*SUM/Q
      G=PI*(Z-68.0)/(2.0*Q)+68.0*ATAN2(Q,FP)/Q+SUM
      G=(4.0*PI*ELCHSQ*(0.0,1.0)/OMEGA)*SQRT(HBAR)/(SQRT(AMASS)*1.41421
     13562)*G
      GBAR=G/SCREEN
      GBAR=GBAR/1.414213562
      GBAR=CONJG(GBAR)*GBAR
      GREAL=REAL(GBAR)
      ALPHA=GREAL
C     INCLUDE FACTOR OF N(0)/(8*PI*FKF**2*Q)*(2*PI)**3
      ALPHA=ALPHA*RHO*PI**2/(Q*FKF**2)
      RETURN
      END
```

LIST OF REFERENCES

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36. Electrons distort a small region of the lattice about their position. It is this virtual phonon cloud which is felt by another electron that forms the attractive mechanism. Normal coulomb repulsion is, of course, still present.

37. The reason that $\bar{g}'$ is indicated instead of g' *is* that the screened electron-phonon coupling constant $\bar{g}$ will be sought self-consistently instead of the bare ion coupling g.

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