POLARON EFFECTS IN THE OPTICAL PROPERTIES OF POLAR SEMI-CONDUCTORS

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ABSTRACT

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by Robert J. Heck

The optical absorption coefficient of a polar semi-conductor is calculated for light energies comparable to the width of the forbidden energy gap of the material in an effort to determine some effects of the electron-phonon interaction. It is expected that the effects will be significant in polar materials because of the strength of the interaction. A simplified version of the Kubo Formula is used which reduces the problem to the calculation of the one-particle electron Green's function. A perturbation approximation is made to determine this function. The result is an absorption coefficient that has anomalous structure occurring at an energy of one phonon above the band edge and a "tail" region of states to which electrons can be excited below the band edge. An improvement is made on the perturbation expansion for the Green's function which results in the appearance of structure at energies of two phonons above the band edge.

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OF POLAR SEMI-CONDUCTORS

By

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I. Introduction

The use of Green's function techniques for performing calculations of the properties of many-body systems is now almost standard. The Green's function formalism has the advantage that it does not require finding the wave functions of the system, which in themselves are rarely of interest anyway.

The one-particle Green's function[1,2,3,4,5] yields information about quantities such as the free energy and density of states of a system and the self-energies and lifetimes of its quasi-particles, and the two-particle Green's function,[1,2,3,4,5] information about transport properties as well as the ground state energy. In this paper we apply Green's function techniques to the calculation of the interband optical absorption coefficient of a polar semi-conducting crystal for photon energies comparable to the band gap. This problem is of interest because the interaction between electrons and longitudinal optical-phonons is significant in these materials and might be expected to lead to observable anomalies in the absorption spectrum.

II. The System Hamiltonian

Associated with the optical-phonon modes in a polar crystal is a dynamic field of dipoles with which the electrons interact. A measure of the strength of this interaction is the coupling constant

$$\frac{e}{\hbar}\left(\frac{m_\ell}{2\hbar}\right)^{1/2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_S}\right)\left(\frac{m}{m_\ell \omega_0}\right)^{1/2} \quad ,$$

, where m is the free electron mass, m_ℓ is the effective mass of a carrier in band ℓ (In our investigation we are interested in transitions from the valence band to the conduction band so the subscript ℓ will refer either to the conduction band, ℓ=c, or to the valence band, ℓ=v.), ϵ_∞ and ϵ_S are the high frequency and static dielectric constants respectively, and ω_0 is a phonon frequency. Values of the coupling constant for various polar substances are shown below.

Table I

LiF 5.2	KCl 5.6	Cu_2O 2.5	PbS 2.5
NaF 6.3	KBr 5.7	MgO 2.3	InSb .014
NaCl 5.5	KI 4.6	ZnO .85	GaAs .06
NaBr 5.0	AgCl 1.7	CdS 1.2	
NaI 4.8	AgBr 1.6	ZnS 1.3	

The interaction energy between an electron and a dipole field is

$$H_{int.} = -\int d^3r\, \vec{D}(r)\cdot\vec{P}(r) \quad ,$$

where $\vec{D}$ is the electric displacement vector of the electron and $\vec{P}$ is the dipole moment per unit volume of the field. From this expression we can see why it is the longitudinal mode rather than a transverse one which interacts most strongly with the electron: integration by parts gives

$$\int \vec{D}\cdot\vec{P}\, d^3r = -\epsilon\int \Phi\ \nabla\cdot\vec{P}\, d^3r \quad ,$$

where $\vec{D}=\epsilon\vec{E}=-\epsilon\nabla\Phi$. But $\nabla\cdot\vec{P}=0$ for a pure transverse mode. The $\vec{D}(r)$ field of a system of electrons having the wave function $\psi(r')$ is

$$-\nabla_r\int e\ \psi^\dagger(r')\,\psi(r')/|r-r'|\ d^3r' \,.$$

For longitudinal phonons $\nabla\times\vec{P} = 0$ so that in this case $\vec{P}$ may be written as the gradient of a scalar potential field $\varphi(r)$, $\vec{P} = \nabla\varphi(r)/4\pi$. Therefore

$$H_{int.} = \frac{e}{4\pi}\int d^3r\, d^3r'\, \nabla_r\left(\frac{\psi^\dagger(r')\,\psi(r')}{|r-r'|}\right)\cdot\nabla_r\varphi(r)$$

$$= -\frac{e}{4\pi}\int d^3r\, d^3r'\, \varphi(r)\nabla^2 \frac{\psi^{+}(r')\,\psi(r)}{|r-r'|}$$

$$= \int d^3r'\, \psi^{+}(r')\,\psi(r')\,\varphi(r') \quad . \qquad (2.1)$$

The first step was an integration by parts; in the last step we used the fact that

$$-\nabla_r^2 \frac{1}{|r-r'|} = \delta(r-r')\,4\pi \quad .$$

The dipole field is related to the longitudinal optical phonons by

$$\vec{P}(r) = \left(\frac{\hbar}{2\mu V\omega_0}\right)^{1/2} \sum_k \frac{\vec{k}}{|k|}\left(b_k^{+} e^{-ik\cdot r} + b_k e^{ik\cdot r}\right),$$

where b_k^{+}, b_k respectively create and annihilate a phonon of momentum k, and since $4\pi\vec{P} = \nabla\varphi$,

$$\varphi(r) = \left(\frac{\hbar}{2\mu V\omega_0}\right)^{1/2} \sum_k \frac{1}{|k|}\left(b_k^{+} e^{-ik\cdot r} - b_k e^{ik\cdot r}\right),$$

where

$$\mu = \frac{4\pi}{\omega_0^2}\left(\frac{\epsilon_\infty \epsilon_s}{\epsilon_s - \epsilon_\infty}\right) \equiv \frac{4\pi}{\omega_0^2}\,\bar{\epsilon} \quad .$$

Inserting the expression for φ in equation (2.1) we obtain the interaction term in the Frohlich Hamiltonian[6]

$$H_{int.} = 4\pi e\left(\frac{\hbar\omega_0}{8\pi\bar{\epsilon}}\right)^{1/2} i \sum_k \frac{1}{|k|} \int d^3r' \, \psi^+(r')\psi(r')$$

$$\times \left(b_k^+ e^{-ik\cdot r'} - b_k e^{ik\cdot r'}\right) \tag{2.2}$$

The total Frohlich Hamiltonian is

kinetic energy of electrons + kinetic energy of phonons

$$+ \int \psi^+(r) V(r) \psi(r) \, d^3r \quad + H_{int.} \tag{2.3}$$

where V(r) is the periodic potential of the crystal lattice when the ions or atomic cores are in their equilibrium positions. If we consider the system to have only one mobile electron, the linear combinations of products of electron wave functions with phonon wave functions which make up the eigenfunctions of this system are said to describe "polarons".

The eigenstates (Bloch states) of the electrons for the Hamiltonian without the interaction term (2.2) are determined, of course, by the structure of the crystal. For convenience we consider a simple structure like a cubic crystal so that quantities like the conductivity will be a constant times the unit tensor. This isotropy implies that the surfaces of constant energy in $\vec{k}$ space are spherical. We further assume that the electrons in the conduction and valence bands have the energy dependence on $\vec{k}$, the quasi-momentum, shown in figure one, i.e., we assume parabolic dispersion curves with the minimum of the conduction band and the maximum of the valence band at $\vec{k} = 0$. So $E(k) = \frac{\hbar^2 k^2}{2m_v}$ and $E(k) = \frac{\hbar^2 k^2}{2m_c} + \Delta$ for valence and conduction electrons respectively, where m_v and m_c are the band masses of the electrons, and Δ is the forbidden energy gap width (note that m_v is negative).

But what are the energy levels of the interacting system? If we assume H int. can be treated as a perturbation then the energy levels will be those of the phonons plus the band electrons plus correction terms obtainable from perturbation theory which are presumably small compared to the first two terms. In addition the Hamiltonian will not mix states of electrons from different bands except in very high orders of perturbation theory. So we can still talk about bands, but of polarons not electrons, and the density of energy states will resemble the non-interacting density of states for electrons in having a forbidden gap.

However the band gap will be "fuzzed out" by the interaction, and the density in the bands will be changed. In the calculation of optical properties of the system, this difference turns out to be important.

III. The Formula for Absorption

To perform the standard calculation for the absorption[7] one takes the first order, time dependent perturbation theory result[8] for the probability of a harmonic external potential of frequency ω to cause a transition in the system from the state j to the state m after a time t:

$$|\langle m|\vec{A}\cdot\vec{p}|j\rangle|^2 \frac{\sin^2(\frac{1}{2}(\omega_{mj}-\omega)t)}{(\hbar(\omega_{mj}-\omega))^2} ,$$

where $\hbar\omega_{mj} = E_m - E_j$, the energy difference between the upper and lower states $\vec{A}$ is the external light potential, and $\vec{p}$ is the momentum operator. To get the total rate one multiplies the above by the probability that in thermal equilibrium m is unoccupied and j is occupied, $N_F(E_m) - N_F(E_j)$ and sums over m and j. Instead of summing one could introduce density of states functions and integrate. This would be a difficult procedure in our case because we would have to calculate the matrix elements and energy levels of the interacting system. Instead we will use a more direct and more exact formal procedure which will require us to find only the one-particle Green's function of the interacting system (but without the exciting light's potential in the Hamiltonian). This formalism due to Kubo[9] is described below.

Our specific goal is to calculate the interband absorption of light by a semi-conducting polar crystal having the previously mentioned simple structure. The absorption coefficient is defined by the equation $I = I_o e^{-\alpha x}$ which relates the intensity I at a distance x into the material to the intensity just inside the surface I_o. Since the absorbed light energy is being taken up by an increase in the kinetic energy of the charge carriers it is not surprising that the absorption is related to the in-phase part of the conductivity; the relation is: $\alpha = \frac{4\pi}{c\epsilon^{1/2}} \mathrm{Re}\,\sigma$;[10] ϵ is the real part of the dielectric constant which can be related to the imaginary part of σ. So if we know $\sigma(\omega)$ we can find all the optical properties[11].

The Kubo formula for conductivity is:

$$\sigma_{ij}(\vec{k},\omega) = \frac{i n e^2}{m\omega}\delta_{ij} + \frac{1}{\hbar\omega}\int_{-\infty}^{\infty} dt \int d^3r\, d^3r'$$

$$\times\ e^{i(\omega t - k\cdot r + k'\cdot r')}\,\theta(t)\left\langle\left[\vec{j}_i(x), \vec{j}_j(x')\right]\right\rangle ,$$

(3.1)

where $t = x_o - x_o'$, N is the average electron density, $\theta(t)$ is a step function, $\langle\ \ \rangle$ means averaging over a grand canonical ensemble i.e. $\langle O\rangle = \frac{Tr e^{-\beta(H - \mu N)}O}{Tr e^{-\beta(H - \mu N)}}$ and

$$\vec{j}(x) = \frac{ie\hbar}{2m}\left\{(\nabla\psi^{+}(x))\,\psi(x) - \psi^{+}(x)\,\nabla\psi(x)\right\}$$

$$- \frac{e^2}{m}\vec{A}(x)\,\psi^{+}(x)\,\psi(x) \qquad ;$$

$\vec{A}(x)$ is the vector potential of the light.

The Kubo formula can be regarded as a consequence of the fluctuation-dissipation theorem[9], which relates general susceptibilities to correlation functions of the related physical response. In this case σ is the susceptibility and $\vec{J}(x)$ is the response. Actually the fluctuation-dissipation theorem can be proved by a generalization of the following derivation of Kubo's formula:

One begins by calculating $\bar{j} = \mathrm{Tr}\rho\vec{j}$, where ρ is the density matrix[12], to first order in the external field, using $\dot{\rho} = it\,[H + \Delta H, \rho]$ where ΔH is the external field part of the Hamiltonian i.e. $\Delta H = -\frac{1}{c}\int dx\, \vec{A}(x) \cdot \vec{j}(x)$. The origin of the two $\vec{j}$'s in $\langle[\vec{j}(x)\vec{j}(x')]\rangle$ in the Kubo Formula is clear at this stage.

It is important to mention that the $\vec{j}(x)$ and $\vec{j}(x')$ operators in the Kubo formula are Heisenberg operators which are developing in time under the full Hamiltonian of the system but without the externally applied field of the exciting light. It is then physically reasonable that $\langle\vec{j}(x)\vec{j}(x')\rangle$, which is a measure of the system's ability to sustain a current without a driving field, should be related to the conductivity.

The quantity $\int \theta(t)\langle[\vec{j}(x), \vec{j}(x')]_-\rangle\, e^{i\omega t}dt$ can be related to a two-particle Green's function as follows:

$$\int \theta(t)\langle[\vec{j}_i(x), \vec{j}_j(x')]_-\rangle\, e^{i\omega t}\, e^{-ik\cdot r}\, e^{ik'\cdot r'}\, dt\, d^3r\, d^3r'$$

$$= \frac{-e^2\hbar^2}{(2m)^2}\int d^3r\, d^3r'\, dt\; \theta(t)\, e^{i\omega t}\, e^{-ik\cdot r}\, e^{ik'\cdot r'}$$

$$\times \langle \{ [(\nabla_i \psi^+(x))\psi(x), (\nabla_j \psi^+(x'))\psi(x')]_-$$

$$- [\psi^+(x)\nabla_i \psi(x), (\nabla_j \psi^+(x'))\psi(x')]_- - [(\nabla_i \psi^+(x))\psi(x), \psi^+(x')\nabla_j \psi(x')]_-$$

$$+ [\psi^+(x)\nabla_i \psi(x), \psi^+(x')\nabla_j \psi(x')]_- \} \rangle \tag{3.2}$$

We have neglected the terms containing $\vec{A}$ in the definition of $\vec{j}$ since the Kubo formula only takes the first power of $\vec{A}$ into account. Also, using the long-wave length approximation, we have replaced $e^{ik\cdot r}$ by 1. We can do an integration by parts on each one of the last three commutators which makes it equal to the first. The quantity (3.2) becomes

$$-\frac{e^2\hbar^2}{m^2} \int d^3r\, d^3r'\, dt\; \theta(t) \langle [(\nabla_i \psi^+(x))\psi(x), (\nabla_j \psi^+(x'))\psi(x')]_- \rangle$$

We choose for our representation of the wave functions the Bloch functions $\eta_{k,\ell}(\vec{x})$ of the non-interacting Hamiltonian (this gives the zero order Green's functions [1,2,3,4,5] a very simple form) i.e. $\psi(x) = \sum_{k,\ell} a_{k,\ell}\,\varphi_{k,\ell}(x)$, $\psi^{\dagger}(x) = \sum_{k,\ell} a^{+}_{k,\ell}\,\varphi^{*}_{k,\ell}(x)$

where $a^{+}_{k,\ell}$ ($a_{k,\ell}$) is an operator in the second-quantized representation which creates (annihilates) an electron of momentum $\vec{k}$ in band ℓ. Equation (3.2) then becomes,

$$-\frac{e^2\hbar^2}{m^2}\int dt\,\theta(t) \sum_{\substack{k_1,k_3\\ \ell_1 \to \ell_4}} v_i(\vec{k},\ell_1,\ell_2)\, v_j(\vec{k},\ell_3,\ell_4)$$

$$\times \left\langle \left[a^{+}_{k_1,\ell_1}(t)\, a_{k_1,\ell_2}(t),\, a^{+}_{k_3,\ell_3}(0)\, a_{k_3,\ell_4}(0) \right]_- \right\rangle ,$$

where

$$v_i(k_1,\ell_1,\ell_2) = \int \nabla_i\, \varphi^{*}_{k_1,\ell_1}(x)\, \varphi_{k_2,\ell_2}(x)\, d^3x \equiv v_i(k_1,k_2,\ell_1,\ell_2)\,\delta_{k_1,k_2} .$$

The delta-function indicates that we are neglecting Umklapp processes.

The quantity

$$\int \theta(t) \left\langle \left[a^{+}_{k_1,\ell_1}(t)\, a_{k_1,\ell_2}(t),\, a^{+}_{k_3,\ell_3}(0)\, a_{k_3,\ell_4}(0) \right]_- \right\rangle e^{i\omega t}\, dt \equiv K_r(\omega) \tag{3.3}$$

can be obtained by calculating the two-particle Green's function

$$\kappa(t) \equiv \langle T(a^{+}_{k_1,l_1}(t)\, a_{k_1,l_2}(t)\, a_{k_3,l_3}(0)\, a_{k_3,l_4}(0))\rangle \quad ,$$

where T is an operator which orders the a's and $a^\dagger$'s from left to right so that those with the latest time arguments are on the left. Time-ordered functions like this one are the Green's functions one calculates by the Matsubara method[1,5] (where the diagram technique is applicable) for imaginary times. It turns out that these imaginary-time functions are periodic along the imaginary axis with period $i/T \equiv i\beta$, where T is now temperature, so that

$$\kappa(\omega_n) = \frac{1}{2}\int_{-\frac{1}{T}}^{\frac{1}{T}} \kappa(t)\, e^{i\omega_n t}\, dt \quad , \quad \omega_n = (2n+1)\pi T \ ,$$

($\kappa(t)$ is an odd function). Then the function we ultimately need, K_r, is related to $\kappa(\omega_n)$ by $K_r(i\omega_n)=\kappa(\omega_n)$ for $\omega_n>0$. So if we can construct a function which is analytic in the upper half of the complex ω-plane and which takes on the values $\kappa(\omega_n)$ at the points $i\omega_n$, we have found $K_r(\omega)$. The above remarks apply to any double-time functions defined analogously to κ and K_r, e.g., consider

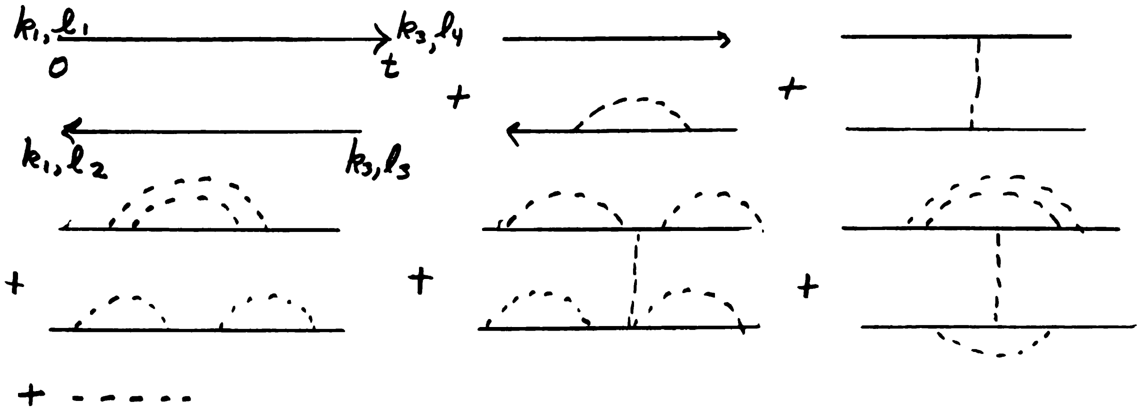
$$G(\vec{k},\omega) = \int \theta(t)\, e^{i\omega t} \langle [a^{+}_{k}(t), a_{k}(0)]_{-} \rangle\, dt$$

and

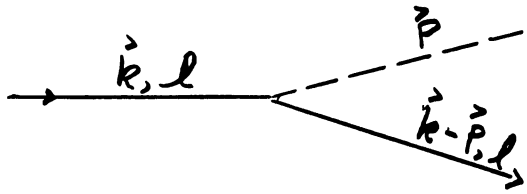
$$\mathcal{G}(k,\omega_n) = \int_{-\frac{1}{T}}^{\frac{1}{T}} e^{i\omega_n t}\langle T(a_k(t)a_k^{+}(0))\rangle\, dt$$

then $G(\vec{k}, i\omega_n) = \mathcal{G}(\vec{k}, \omega_n)$.

Now we have transformed the problem to the calculation of a two-particle Green's function, but we will go further and reduce the two-particle function to a product of one-particle functions by an approximation which is valid for our particular system[13,14]. The reason for this step is that better techniques are available for calculating one-particle functions than for two-particle functions. To perform this reduction we note first that transitions in which $\ell_1=\ell_2$ and/or $\ell_3=\ell_4$ refer to intra-band transitions which we are not considering. Then the diagrams for $\kappa(t)$ take the form



where the solid lines are electron propagators, the dotted lines are phonon propagators, and the vertices are interactions in which $\vec{k}$ and ℓ are conserved, i.e.

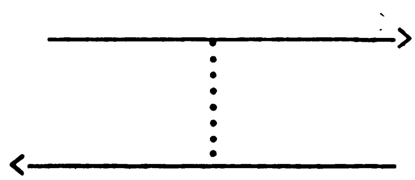


.

Also the propagators are diagonal in $\vec{k}$ and ℓ i.e.

$$\langle T(a^{+}_{k_1 \ell_1}(t)\, a_{k_1 \ell_1}(0))\rangle = G_0(\vec{k}_1, \ell_1)\, \delta_{k_1 k_2}\, \delta_{\ell_1 \ell_2}$$

so $\ell_1 = \ell_4 \neq \ell_2 = \ell_3$. Then the diagrams show an electron in one band going from 0 to t and a second electron in the other band going from t to 0, or equivalently, a hole in this band going from 0 to t. Both electrons have interactions with themselves and each other via the phonons. Consider the simplest process in which the two electrons interact with each other i.e. one in which they exchange a single phonon as denoted by this diagram:



The "asymptotic theorem" due to Bonch-Bruevich[13,14] states that in the set of all diagrams which must be summed to find the two-particle Green's function, the sum of those diagrams, such as the above, which contain phonon propagators connecting the propagators for the two distinct electrons, is negligible if the band-gap energy is much greater than the energy of a phonon, $\Delta \gg \hbar\omega_0$. The proof of the theorem apparently depends on showing that matrix elements of interactions such as the one taking place in our simple diagram are small. According to the Feynman rules[1,5] for evaluating this diagram, the following factor enters into the amplitude for this process:

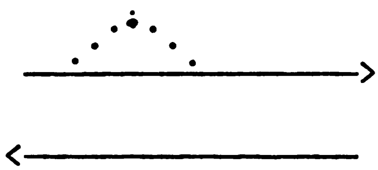
$$\sum_{k_1} \int d^3r_1\, d^3r_2\; \psi^+_{k,c}(r_1)\,\psi_{k-k_1,c}(r_1)\;\psi^+_{k',v}(r_2)\,\psi_{k'+k_1,v}(r_2)\;\frac{e^{ik_1\cdot(r_1-r_2)}}{|k_1|^2}$$

$$\longrightarrow \int \frac{\psi^+_{k,c}(r_1)\,\psi_{k-k_1,c}(r_1)\,\psi^+_{k',v}(r_2)\,\psi_{k'+k_1,v}(r_2)}{|r_1-r_2|}\; d^3r_1\, d^3r_2$$

(We have chosen the electron at r_1 to be in the conduction band and the electron at r_2 to be in the valence band).
Due to the fact that electrons in the valence band are predominantly closer to the ions or atomic cores than electrons in the conduction band, there may be some basis for saying this integral is smaller than one like

$$\int \left(\psi^+_{k,c}(r)\,\psi_{k-k_1,c}(r)\;\psi^+_{k',c}(r')\,\psi_{k'+k_1,c}(r')\;\phi(|r-r'|)\right) d^3r\, d^3r'$$

which is a factor in a diagram such as



since there should be more overlap of the functions in the integrand of the latter expression. However, I know of no convincing general proof of the inequality, so that the "asymptotic theorem" may not really be a theorem, although I expect it to be valid in many cases and as we shall see later, it leads to a reasonable result. If we follow Bonch-Bruevich and assume the "asymptotic theorem", we see that in the set of diagrams for $\kappa(\omega)$ we can neglect those which connect the two solid electron propagator lines with a dotted phonon propagator line. Then $\kappa(\omega)$ becomes the Green's function for independent propagation of an electron in band ℓ_1 from 0 to t and an electron in band ℓ_2 from t to 0, i.e. $\kappa(t) \dashrightarrow \mathcal{G}(\vec{k}_1, \ell_1, t) \times \mathcal{G}(\vec{k}_1, \ell_2, -t)$ or

$$K(\omega_n) = \frac{1}{2}\int_{-1/T}^{1/T} e^{i\omega_n t}\, \mathcal{G}(k_1, \ell_1, t)\, \mathcal{G}(k_1, \ell_2, -t)\, dt$$

$$= \frac{1}{2}\int e^{i\omega_n t}\, T^2 \sum_{n', n''} \mathcal{G}(k_1, \ell_1, \omega_{n'})\, \mathcal{G}(k_1, \ell_2, \omega_{n''})\, e^{i\omega_{n'} t} e^{-i\omega_{n''} t}\, dt$$

$$= T \sum_{n',n''} \mathcal{G}(k_1,l_1,\omega_{n'})\, \mathcal{G}(k_2,l_2,\omega_{n''})\, \delta(\omega_n+\omega_{n'}-\omega_{n''})$$

$$= T \sum_{n'} \mathcal{G}(k_1,l_1,\omega_{n'})\, \mathcal{G}(k_1,l_2,\omega_n+\omega_{n'})$$

To do this summation we take advantage of the residue theorem in the theory of complex variables, using the fact that the function $1/e^{\beta\omega'}+1$ has singularities at $\omega'=(2n+1)i\pi T$ and residues at these points equal to $1/T\equiv\beta$. To apply this method we must know what the continuation of $\mathcal{G}$ is in the complex ω' space. As explained already for double-time Green's functions, there exists a function $G_r(\omega)$ such that $G_r(i\omega_n)=\mathcal{G}(\omega_n)$, $\omega_n>0$ where

$$G_r(t) = -i\langle[\psi(t),\psi^+(0)]_-\rangle\,\theta(t)\ .$$

Similarly there exists a function $G_a(\omega)$ such that $G_a(i\omega_n)=\mathcal{G}(\omega_n)$, $\omega_n>0$, where

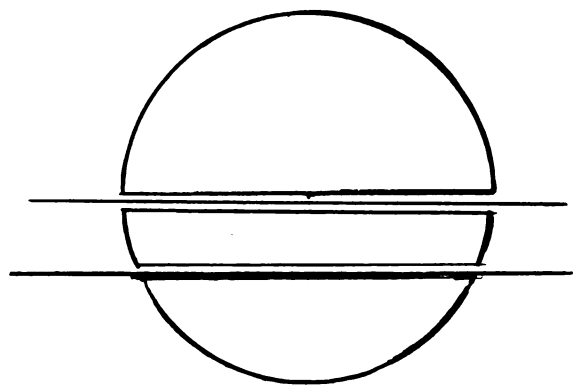
$$G_a(t) = -i\langle[\psi(t),\psi^+(0)]_-\rangle\,\theta(-t)\ .$$

$G_r(\omega)$ is analytic in the upper half-plane; $G_a(\omega)$ is analytic in the lower half-plane; so the summation becomes:

$$T\sum_{n'} \mathcal{G}(k_1,l_1,\omega_{n'})\,\mathcal{G}(k_1,l_2,\omega_n+\omega_{n'})$$

$$\rightarrow \int \frac{G_{r/a}(k_1,l_1,\omega')\,G_{r/a}(k_1,l_2,\omega'+i\omega_n)}{e^{\beta\omega'}+1}\,d\omega'$$

where the integration is over this contour:



The contour avoids all the singularities of the integrand except those at $\omega=(2n+1)i\pi T$ (there are other singularities since the first function in the integrand changes from G_r to G_a at the line Im $\omega'=0$, and the second function in the integrand changes from G_r to G_a at the line Im $\omega'=-i\omega_n$); so the residue theorem assures us that the integral equals the summation. Since the contributions to the integral associated with the arcs at infinity are zero, the four horizontal lines are the only part of the contour that require consideration.

$$K(\omega) \sim \int_{-\infty}^{\infty} d\omega' \left\{ \frac{G_r(k_1, l_2, \omega' + i\omega_n)}{e^{\beta\omega'}+1} \right.$$

$$\times \left[G_r(k_1, l_1, \omega') - G_A(k_1, l_1, \omega') \right] + \frac{G_a(k_1, l_1, \omega' - i\omega_n)}{e^{\beta(\omega' - i\omega_n)}+1}$$

$$\left. \times \left[G_r(k_1, l_2, \omega') - G_a(k_1, l_2, \omega') \right] \right\} =$$

$$2\int_{-\infty}^{\infty} d\omega' \left\{ \frac{G_r(k_1, l_2, \omega' + i\omega_n)}{e^{\beta\omega'}+1} \operatorname{Im} G_r(k_1, l_1, \omega') \right.$$

$$\left. + \frac{G_a(k_1, l_1, \omega' - i\omega_n)}{e^{\beta(\omega' - i\omega_n)}+1} \operatorname{Im} G_r(k_1, l_2, \omega') \right\} .$$

(We have used the fact that $G_r(\omega) = G_a^*(\omega)$ which follows from the definitions of $G_r(t)$ and $G_a(t)$.) Since

$$e^{\beta(\omega' - i\omega_n)} = e^{\beta(\omega' - i(2n+1)\pi T} = e^{\beta\omega'} ,$$

$$K(\omega) = 2\int_{-\infty}^{\infty} d\omega' \left\{ \frac{G_r(k_1, l_2, \omega' + i\omega_n)}{e^{\beta\omega'}+1} \operatorname{Im} G_r(k_1, l_1, \omega') \right.$$

$$+ \frac{G_a(k_1,l_1,\omega'-i\omega_n)}{e^{\beta(\omega'-i\omega_n)}+1} \operatorname{Im} G_r(k_1,l_2,\omega') \Big\} \quad .$$

Then since Im $K_r(i\omega_n)$=Im $\kappa(\omega_n)$ we find:

$$\operatorname{Im} K_r(\omega) = 2\int_{-\infty}^{\infty} \Big\{ \operatorname{Im} G_r(k_1,l_1,\omega') \frac{\operatorname{Im}}{e^{\beta\omega'}+1} G_r(k_1,l_2,\omega+\omega')$$

$$- \operatorname{Im} G_r(k_1,l_1,\omega'-\omega) \frac{\operatorname{Im}}{e^{\beta\omega'}+1} G_r(k_1,l_2,\omega') \Big\} \quad ,$$

and finally letting $\omega+\omega'\longrightarrow\omega'$ in the first term we obtain:

$$\operatorname{Im} K_r(\omega) = 2\int_{-\infty}^{\infty} d\omega' \operatorname{Im} G_r(k_1,l_2,\omega') \operatorname{Im} G_r(k_1,l_1,\omega'-\omega)$$

$$\times \left(n_F(\omega'-\omega) - n_F(\omega')\right) \quad ,$$

where $n_f(\omega')=1/e^{\beta\omega'}+1$.

Thus the Kubo Formula (3.1) becomes

$$\alpha(\omega) = \frac{4\pi}{c\epsilon^{1/2}} \operatorname{Re}\sigma(\omega) = \frac{2e^2}{c\epsilon^{1/2}\pi m} \int d^3k\, dE \sum_{\substack{l=c,v\\ l'=c,v\\ l\neq l'}}$$

$$v_i(\vec{k},l,l')\, v_j(\vec{k},l,l')\, \operatorname{Im} G_r(\vec{k},l,E-\omega)\left(n_F(E-\omega)-n_F(E)\right)$$

$$= \frac{2e^2\, v_i\, v_j}{\hbar\omega c\epsilon^{1/2}\pi m} \int d^3k\, dE \Big\{ \operatorname{Im} G_r(\vec{k},c,E-\omega)$$

$$\times \operatorname{Im} G_r(\vec{k},v,E) + \operatorname{Im} G_r(\vec{k},E-\omega) \operatorname{Im} G_r(\vec{k},c,E)\Big\}$$

$$\left(n_F(E-\omega) - n_F(E)\right) .$$

The first term will give practically no contribution because $\operatorname{Im} G_r(\vec{k},c,E-\omega)$ is peaked at a distance $2\Delta-u$ from $\operatorname{Im} G_r(\vec{k},v,E)$, as we will see later when we get an explicit expression for G_r.

At this time we make the replacement $v_i v_j \longrightarrow 1/3 \times \Sigma_i \; |\langle \ell | v_i | \ell' \rangle|^2 \equiv |v(\vec{k})|^2$, which is valid for a cubic crystal. Also we assume that $v(\vec{k})$ is slowly varying with $\vec{k}$ so we can take it out of the integrand. Then we obtain the final form of the expression for α:

$$\alpha(\omega) = \frac{2e^2 |v(\vec{k})|^2}{c\,\epsilon^{1/2}\pi m \omega} \int d^3k \, dE \;\; \mathrm{Im}\, G_r(\vec{k}, V, E-\omega)$$

$$\times \, \mathrm{Im}\, G_r(\vec{k}, c, E) \;\; \left(n_F(E-\omega) - n_F(E)\right) \tag{3.4}$$

In the limit as the electron-lattice interaction goes to zero,

$$\mathrm{Im}\, G_r(\vec{k}, \ell, E) \rightarrow \frac{1}{(2\pi)^4} \, \delta\left(E - \frac{\hbar^2 k^2}{2m_\ell} - \Delta\, \delta_{\ell c} + \mu\right) ,$$

and the expression becomes the one which is well-known for inter-band absorption[15]: $\alpha(\omega) \sim (\hbar\omega - \Delta)^{1/2}$. Less trivially the formula for α begins to look like the one described earlier as the "standard approach" if one observes that Im $G_r(\ell, \vec{k}, \omega)$ is the density of states for a given $\vec{k}$ and ω in band ℓ. In that formulation one has a product of a squared matrix element between initial and final states, the density of states at the initial state, the density of states at the final state, and the thermal probability that the initial state is occupied and the final state is unoccupied. Then one sums this quantity over all initial and final states(ρ is the density of states):

$$\alpha(\omega) \sim \int d^3k_i\, d^3k_f\, dE_i\, dE_f\, M^2 \rho(k_i, E_i)\, \rho(k_f, E_f)(n_F(i) - n_F(f))$$

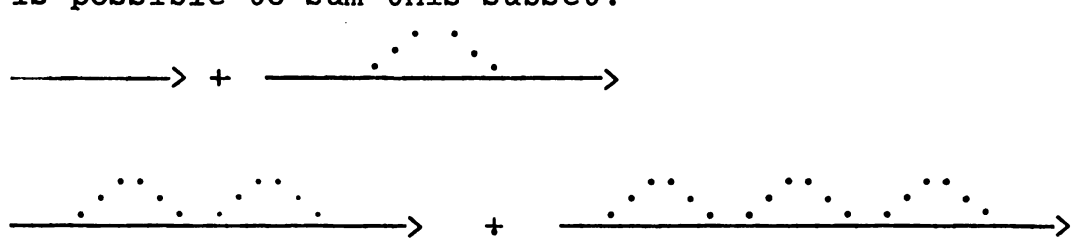
Conservation of energy and momentum causes the above to reduce to:

$$\alpha(\omega) \sim \int d^3k\, dE\, M^2 \rho(\vec{k}, E)\, \rho(\vec{k}, E-\omega)(n_F(i) - n_F(f))$$

which agrees with our final form of the Kubo Formula after the substitution of $\rho(\vec{k},E)$ for Im $G_r(\vec{k},E)$. It is shown in textbooks on Green's functions[1,2,3] that Im G_r is indeed the density of states of the normal modes of an interacting system.

IV. The One-Particle Green's Function

The main task left is to calculate the one-particle Green's function. It is the sum of all the connected self-energy diagrams[1,5]; it is impossible to sum all the diagrams, but it is possible to sum this subset:



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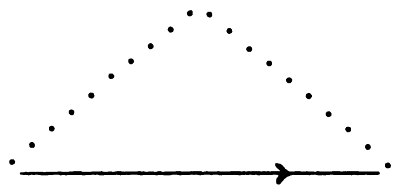
where the solid lines are electron propagators, dotted lines are phonon propagators, and the vertices are interactions as in the two particle diagrams. To generate this subset one calculates the self energy, $\Sigma(k,\omega)$ corresponding to this diagram:



and inserts it into the Dyson' equation

$$\mathcal{G}(\vec{k},\ell,\omega) = 1 / \mathcal{G}_0^{-1}(\vec{k},\ell,\omega) - \Sigma(\vec{k},\ell,\omega) ,$$

where $\mathcal{G}_0$ is the free electron propagator $\frac{\hbar}{i\hbar\omega - E_0(k,\ell) + \mu}$ and $E_0(k,\ell)$ is the energy of a free electron in the ℓth band. The Dyson equation can be written alternatively as

$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$, which can be solved for a given Σ in a perturbation sense by iteration, giving:

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}_0 \Sigma \mathcal{G}_0 + \cdots ,$$

which explains how our subset is generated by Dyson's equation. According to the Feynman rules

$$\Sigma(\vec{p},\ell,\omega_n) = \frac{e^2\omega_0}{4\pi^2\hbar\bar{\epsilon}} T \sum_{\omega_{n'}} \int \frac{d^3k}{|k|^2} G_0(\vec{p}-\vec{k},\ell,\omega_n-\omega_{n'}) D_0(\vec{k},\omega_{n'}) ;$$

if we let temperature be low,

$$T\sum_{\omega_{n'}} \to \frac{1}{2\pi}\int d\omega' \,, \quad \Sigma(\vec{P},\omega_n) \to \frac{c^2\omega_0 \hbar}{8\pi^3\hbar\epsilon}\int \frac{d^3k\, d\omega'}{|k|^2}$$

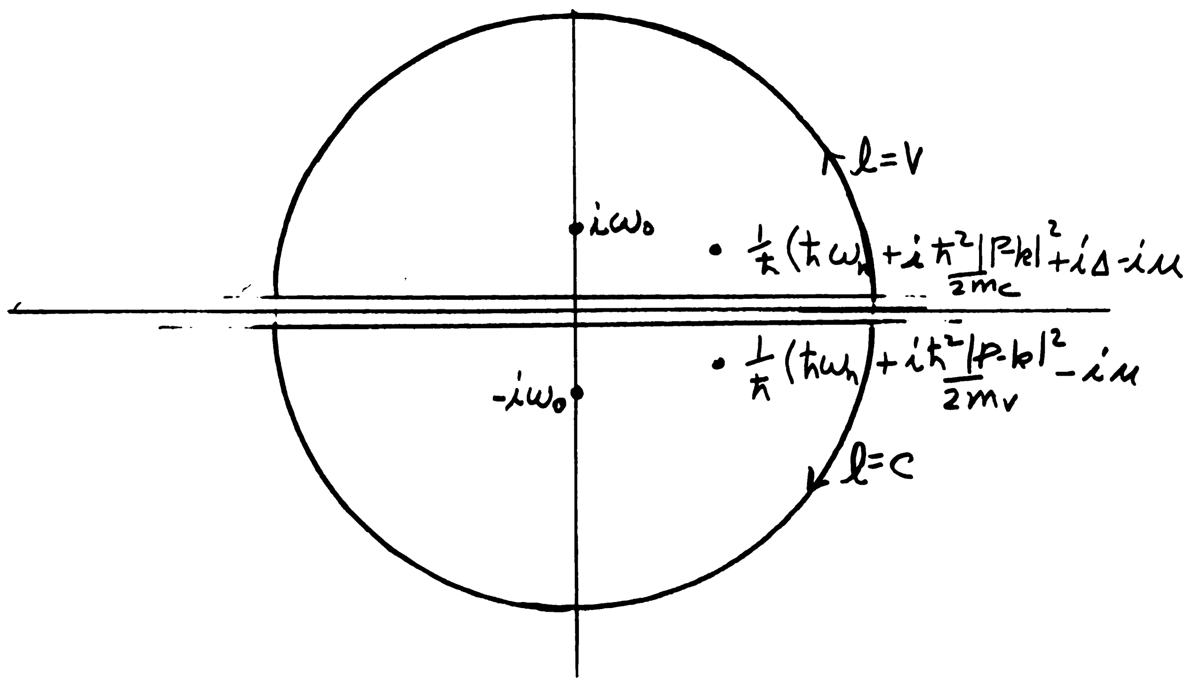
$$\frac{\frac{i}{2}\left(\frac{1}{\omega'-i\omega_0} - \frac{1}{\omega'+i\omega_0}\right)}{i\hbar(\omega_n-\omega') - \frac{\hbar^2}{2m_\ell}|\vec{P}-\vec{k}|^2 - \Delta\delta_{\ell,c} + \mu} \, .$$

ω' integration:

The poles of the integrand are at $\omega' = \pm i\omega_0$,

and $\omega' = \frac{1}{\hbar}\left(\hbar\omega_n + i\frac{\hbar^2}{2m_\ell}|\vec{P}-\vec{k}|^2 + i\Delta\delta_{\ell,c} - i\mu\right)$

The last pole is in upper (lower) half-plane if ℓ = c(v), whichever is the case we close the contour to include only one pole as in the diagram.



$$\Sigma(\vec{p},\ell,\omega_n) = -\frac{e^2\omega_0}{8\pi^3\bar{\epsilon}} \int \frac{d^3k}{|k|^2} \frac{1}{i\hbar\omega_n \mp \hbar\omega_0 - \frac{\hbar^2}{2m_\ell}|\vec{p}-\vec{k}|^2 - \Delta\delta_{\ell,c} + \mu}$$

(upper sign for ℓ=c, lower for ℓ=v). Introducing spherical coordinates and letting the polar axis lie along the $\vec{p}$ vector we obtain,

$$\Sigma = \frac{e^2\omega_0}{4\pi\bar{\epsilon}} \int \frac{dk\, d\theta \sin\theta}{i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{\ell,c} + \mu - \frac{\hbar^2}{2m_\ell}(p^2+k^2-2pk\cos\theta)}$$

$$= \frac{e^2\omega_0}{4\pi\bar{\epsilon}} \frac{m_\ell}{\hbar^2 p} \int \frac{dk}{k} \ln\left|\frac{i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{\ell,c} + \mu - (\hbar^2/2m_\ell)(p^2+k^2+2pk)}{i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{\ell,c} + \mu - (\hbar^2/2m_\ell)(p^2+k^2-2pk)}\right|$$

$$= \frac{e^2\omega_0}{4\pi\bar{\epsilon}} \frac{m_\ell}{\hbar^2 p} \int_0^\infty \frac{dk}{k} \ln\left|\frac{i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{\ell,c} + \mu - (\hbar^2/2m_\ell)(p+k)^2}{i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{\ell,c} + \mu - (\hbar^2/2m_\ell)(p-k)^2}\right|$$

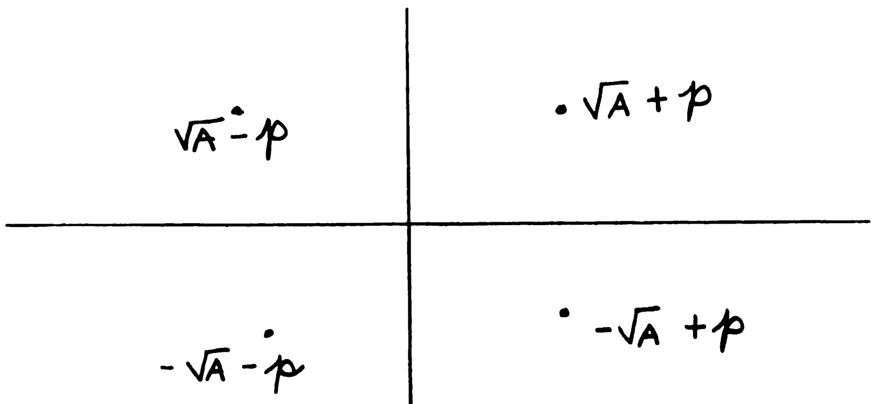
$$\sim \int_0^\infty \frac{dk}{k} \ln\left|\frac{A-(p+k)^2}{A-(p-k)^2}\right|$$

$$A = \frac{2m_l}{\hbar^2}\left(i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{l,c} + \mu\right)$$

Since the integrand is odd, the above integral equals

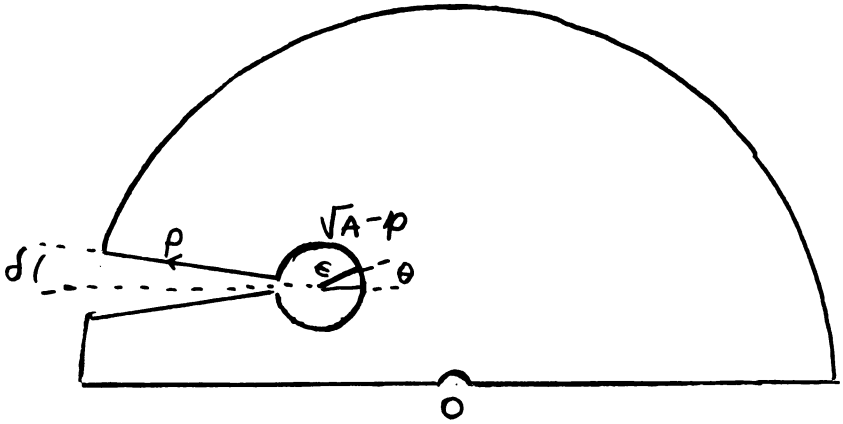
$$\frac{1}{2}\int_{-\infty}^{\infty}\frac{dk}{k}\,\ln\left|\frac{A-(p+k)^2}{A+(p-k)^2}\right| = \frac{1}{2}\int_{-\infty}^{\infty}\frac{dk}{k}\Big(\ln\left|\sqrt{A}-(p+k)\right|$$

$$+\ln\left|\sqrt{A}+(p+k)\right| - \ln\left|\sqrt{A}+(p-k)\right| - \ln\left|\sqrt{A}-(p-k)\right|\Big)$$



(position of poles in complex k-plane)

If we close the contour in the upper plane the first and third terms in the above integrand have singularities that must be avoided. For the first term the contour is:



We always avoid the k = 0 pole because our derivation of the interaction Hamiltonian implicitly assumed that the summation over $\vec{k}$ did not include $\vec{k} = 0$. Since the integrand vanishes on the arc and is analytic inside the contour the first term equals:

$$\int_M \frac{dk}{k} \ln|\sqrt{A}-p-k| = \lim_{\delta\to 0}\int_\infty^0 d\rho\, e^{i(\pi-\delta)} \times \frac{\ln\rho + i(\pi-\delta)}{\rho e^{i(\pi-\delta)}+\sqrt{A}-p} + \int_0^\infty d\rho\, e^{i(\delta-\pi)} \times \frac{\ln\rho+i(\delta-\pi)}{\rho e^{i(\delta-\pi)}+\sqrt{A}-p} + \lim_{\epsilon\to 0}\int_{\delta-\pi}^{\pi-\delta} i\epsilon \frac{(\ln\epsilon+i\theta)\,d\theta}{\epsilon e^{i\theta}+\sqrt{A}-p},$$

where M is the key-hole-like part of the above contour.

The last integral has a uniformly continuous integrand so we can exchange the order of the integration and taking the limit as $\epsilon \longrightarrow 0$. The only part that may give trouble is

$$\lim_{\epsilon \to 0} \frac{\epsilon \ln \epsilon \, e^{i\theta}}{\sqrt{A} - p + \epsilon e^{i\theta}} = \lim_{\epsilon \to 0} \frac{\epsilon \ln \epsilon \, e^{i\theta}}{\sqrt{A} - p}$$

But $\lim_{\epsilon \to 0} \epsilon \ln \epsilon = 0$, so the last integral is zero. The first two integrals add up to

$$2\int_0^\infty \frac{e^{i\pi}(-i\pi)\, d\rho}{\rho e^{i\pi} + \sqrt{A} - p} = 2\int_0^\infty \frac{i\pi \, d\rho}{-\rho + \sqrt{A} - p}$$

$$= -2\pi i \ln|\sqrt{A} - p - \rho| \Big|_0^\infty = \lim_{\rho \to \infty} \ln|A - p - \rho|$$

$$+ 2\pi i \ln|\sqrt{A} - p|$$

A similar calculation shows that the singularity at $\sqrt{A} + p$ in the third term of Σ gives

$$-\left(-2\pi i \lim_{\rho \to \infty} \ln|\sqrt{A} + p - \rho| + 2\pi i \ln|\sqrt{A} + p|\right);$$

so

$$\Sigma \sim 2\pi i \lim_{\rho\to\infty} \left(\ln\left|\frac{\sqrt{A}-p}{\sqrt{A}+p}\right| - \ln\left|\frac{\sqrt{A}+p-\rho}{\sqrt{A}-p-\rho}\right| \right)$$

The last term approaches the log of unity, which is zero, so that

$$\Sigma(\vec{p},l,\omega_n) = \frac{i e^2 \omega_0 m_l}{2\hbar^2 \bar{\epsilon}\, p} \ln\left| \frac{\left(\frac{2m_l}{\hbar^2}(i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{l,c} + \mu)\right)^{\frac{1}{2}} - p}{\left(\frac{2m_l}{\hbar^2}(i\hbar\omega_n \mp \hbar\omega_0 - \Delta\delta_{l,c} + \mu)\right)^{1/2} + p} \right|$$

Let $\frac{i e^2 \omega_0 m_l}{2\hbar^2 \bar{\epsilon}} \equiv i g_l^2$, then

$$\mathcal{G}(\vec{p},l,\omega_n) = \hbar \Big/ i\hbar\omega_n - \frac{\hbar^2 p^2}{2m_l} - \Delta\delta_{l,c} + \mu - \Sigma(\vec{p},l,\omega_n)$$

and

$$G_r(\vec{p},l,\omega) = \hbar \Big/ \hbar\omega - \frac{\hbar^2 p^2}{2m_l} - \Delta\delta_{l,c} + \mu - \Sigma(\vec{p},l,-i\omega)$$

for ω in the upper half complex ω-plane. Note that $G_r(i\omega_n) = \mathcal{G}(\omega_n)$ as required.

V. The Absorption Curve

At low temperatures the factor $N_f(E-\hbar\omega)-N_f(E)$ in the Kubo Formula equals unity if $\hbar\omega$ is of the order of the band-gap. The Kubo Formula for the absorption (3.4) is now,

$$\alpha(\omega) = \frac{2e^2|U(k)|^2}{c\,\epsilon^{1/2} m\,\omega} 4\pi \int dk\, k^2\, dE$$

$$\times \operatorname{Im}\left(1\Big/ E-\hbar\omega-\frac{\hbar^2 k^2}{2m_v}+\mu+i\frac{g_v^2\hbar}{k}\ln\left|\frac{\left(\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{1/2}+k}{\left(\quad '' \quad\right)^{1/2}-k}\right| \right)$$

$$\times \operatorname{Im}\left(1\Big/ E-\frac{\hbar^2 k^2}{2m_c}-\Delta+\mu+i\frac{g_c^2\hbar}{k}\ln\left|\frac{\left(\frac{2m_c}{\hbar^2}(E-\hbar\omega_0-\Delta+\mu)\right)^{1/2}+k}{\left(\quad '' \quad\right)^{1/2}-k}\right| \right) \tag{5.1}$$

We have gone to spherical coordinates and integrated over the angles. This merely introduced a factor of 4π, since the integrand did not depend on the angles. If $E>\hbar\omega-\hbar\omega_0-\mu$ the log in the first term in α has the form

$$\ln\left|\frac{ia+b}{ia-b}\right| \qquad \text{where } a,b \text{ are real.}$$

$$\ln\left|\frac{ia+b}{ia-b}\right| = \ln(a^2+b^2) + i\tan^{-1} a/b - \ln(a^2+b^2)$$

$$-i\tan^{-1}(-a/b) = 2i\tan^{-1} a/b \quad .$$

Then the first factor in α is,

$$\mathrm{Im}\ 1\Big/ E-\hbar\omega+i\epsilon-\frac{\hbar^2 k^2}{2m_v}-2\frac{g_v^2\hbar}{k}\tan^{-1}\left(\frac{\left(-\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{1/2}}{k}\right).$$

The $i\epsilon$ factor is there because G_r is the analytic continuation of $\mathcal{G}$ in the upper half of the complex ω -plane. Using the fact that

$$\lim_{\epsilon\to 0}\frac{1}{x+i\epsilon} = P\frac{1}{x} + i\pi\delta(x) \quad ,$$

where P means Cauchy principal value we find the above factor is

$$\pi\,\delta\left(E-\hbar\omega-\frac{\hbar^2 k^2}{2m_v}-2\frac{g_v^2\hbar}{k}\tan^{-1}\left(\frac{\left(-\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{1/2}}{k}\right)\right).$$

By a similar analysis we find that the second factor becomes

$$\pi\,\delta\left(E-\frac{\hbar^2k^2}{2m_c}-\Delta+\mu-\frac{g_c^2\hbar}{k}\,2\tan^{-1}\left(\frac{\left(-\frac{2m_c}{\hbar^2}(E-\hbar\omega_0-\Delta+\mu)\right)^{1/2}}{k}\right)\right).$$

when $E<\Delta+\hbar\omega_0-\mu$

So

$$\int dk\,dE\,\mathrm{Im}\,G_r(\vec{k},v,E-\hbar\omega)\,\mathrm{Im}\,G_r(\vec{k},c,E)$$

$$\sim\pi\int_0^{\hbar\omega-\hbar\omega_0} dk\,dE\,k^2\,\mathrm{Im}\,\frac{1}{E-\hbar\omega-\frac{\hbar^2k^2}{2m_v}+i\frac{g_v^2\hbar}{k}\ln\left|\frac{\left(\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{1/2}+k}{\left(\quad''\quad\right)^{1/2}-k}\right|}$$

$$\times\,\delta\left(E-\frac{\hbar^2k^2}{2m_c}-\Delta-\frac{g_c^2\hbar}{k}\,2\tan^{-1}\left(\frac{\left(-\frac{2m_c}{\hbar^2}(E-\hbar\omega_0-\Delta+\mu)\right)^{1/2}}{k}\right)\right)$$

$$+\,\pi^2\int_{\hbar\omega-\hbar\omega_0}^{\Delta+\hbar\omega_0} dk\,dE\,k^2\,\delta\left(E-\hbar\omega-\frac{\hbar^2k^2}{2m_v}-\frac{g_v^2\hbar 2}{k}\tan^{-1}\left(\frac{\left(-\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{1/2}}{k}\right)\right)$$

$$\times\,\delta\left(E-\frac{\hbar^2k^2}{2m_c}-\Delta+\mu-2\frac{g_c^2\hbar}{k}\tan^{-1}\left(\frac{\left(-\frac{2m_c}{\hbar^2}(E-\hbar\omega_0-\Delta+\mu)\right)^{1/2}}{k}\right)\right)$$

$$+\pi\,\delta\left(E-\hbar\omega-\frac{\hbar^2k^2}{2m_v}+\mu-2g_v^2\frac{\hbar}{k}\tan^{-1}\left(\frac{\left(-\frac{2m_v}{\hbar^2}(E-\hbar\omega+\hbar\omega_0+\mu)\right)^{\frac{1}{2}}}{k}\right)\right)$$

$$\times\,\mathrm{Im}\,\frac{1}{E-\frac{\hbar^2k^2}{2m_c}-\Delta+\mu+i g_c^2\frac{\hbar}{k}\ln\left|\frac{\left(\frac{2m_c}{\hbar^2}(E-\hbar\omega_0-\Delta+\mu)\right)^{\frac{1}{2}}+k}{\left(\quad '' \quad\right)^{\frac{1}{2}}-k}\right|}\,.$$

The first term is zero unless

$$\hbar\omega-\hbar\omega_0-\mu>\Delta+\frac{\hbar^2k^2}{2m_c}-\mu+g_c^2\frac{\hbar}{k}2\tan^{-1}\left(\frac{\left(\frac{2m_c}{\hbar^2}(\hbar\omega_0+\Delta-E-\mu)\right)^{\frac{1}{2}}}{k}\right).$$

The second term is zero unless

$$\Delta+\hbar\omega_0-\mu>\hbar\omega+\frac{\hbar^2k^2}{2m_v}-\mu+2g_v^2\frac{\hbar}{k}\tan^{-1}\left(\frac{\left(\frac{2m_v}{\hbar^2}(\hbar\omega-E-\hbar\omega_0-\mu)\right)^{\frac{1}{2}}}{k}\right)$$

$$>\hbar\omega-\hbar\omega_0-\mu,$$

and

$$\Delta+\hbar\omega_0-\mu>\frac{\hbar^2k^2}{2m_c}+\Delta-\mu-2g_c^2\frac{\hbar}{k}\tan^{-1}\left(\frac{\left(\frac{2m_c}{\hbar^2}(\Delta+\hbar\omega_0-E-\mu)\right)^{\frac{1}{2}}}{k}\right)$$

$$>\hbar\omega-\hbar\omega_0-\mu\,.$$

The third term is zero unless

$$\infty>\hbar\omega+\frac{\hbar^2k^2}{2m_v}-\mu+2g_v^2\frac{\hbar}{k}\tan^{-1}\left(\frac{\left(\frac{2m_v}{\hbar^2}(\hbar\omega-E-\hbar\omega_0-\mu)\right)^{\frac{1}{2}}}{k}\right)$$

$$>\Delta+\hbar\omega_0-\mu\,.$$

The above restrictions determine the k limits after the E integration is done, however, it is necessary to simplify the above expressions to determine these limits so we will neglect the terms which are small because they contain g_v and g_c. This causes a small error in the determination of the ranges over which the three terms in the expression for the absorption are non-zero. The integral becomes

$$\pi^2\int_{\left(\frac{-2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}}^{\left(\frac{2m_c\hbar\omega_0}{\hbar^2}\right)^{1/2}} k^2\,dk\,\delta\Bigg(\frac{\hbar^2k^2}{2m_c}+\Delta-\hbar\omega-\frac{\hbar^2k^2}{2m_v}-\frac{2g_c^2\hbar}{k}\tan^{-1}\left(\frac{\left(\frac{2m_c}{\hbar^2}\left(\hbar\omega_0+\frac{\hbar^2k^2}{2m_v}\right)\right)^{1/2}}{k}\right)$$

$$-\frac{2g_v^2\hbar}{k}\tan^{-1}\left(\frac{\left(\frac{2m_v}{\hbar^2}\left(\hbar\omega-\Delta-\hbar\omega_0-\frac{\hbar^2k^2}{2m_c}\right)\right)^{1/2}}{k}\right)\Bigg)$$

$$+\int_{\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}}^{\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}} dk\;k^2\qquad\times$$

$$\times \operatorname{Im} \frac{1}{\hbar\omega - \Delta - \frac{\hbar^2 k^2}{2m_c} + \frac{\hbar^2 k^2}{2m_v} - i\frac{g_v^2 \hbar}{k} \ln\left| \frac{\left(\frac{2m_v}{\hbar^2}\left(\frac{\hbar^2 k^2}{2m_v} + \hbar\omega_0\right)\right)^{1/2} + k}{\left(\qquad '' \qquad\right)^{1/2} - k} \right| \quad +}$$

$$\overline{\quad + i\frac{g_c^2 \hbar}{k} \ln\left| \frac{\left(\frac{2m_c}{\hbar^2}\left(\hbar\omega + \frac{\hbar^2 k^2}{2m_v} - \hbar\omega_0 - \Delta\right)\right)^{1/2} + k}{\left(\qquad '' \qquad\right)^{1/2} - k} \right|}$$

$$+ \pi \int_0^{\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0)\right)^{1/2}} dk\, k^2 \left(\operatorname{Im} \frac{1}{\hbar\omega - \Delta - \frac{\hbar^2 k^2}{2m_v} + \frac{\hbar^2 k^2}{2m_c} - i\frac{g_v^2 \hbar}{k} \ln\left| \frac{\left(\frac{2m_v}{\hbar^2}\left(\hbar\omega_0 + \frac{\hbar^2 k^2}{2m_v}\right)\right)^{1/2} + k}{\left(\qquad '' \qquad\right)^{1/2} - k} \right| +} \right.$$

$$\overline{\quad + i\frac{g_c^2 \hbar}{k} \ln\left| \frac{\left(\frac{2m_c}{\hbar^2}\left(\hbar\omega + \frac{\hbar^2 k^2}{2m_v} - \hbar\omega_0 - \Delta\right)\right)^{1/2} + k}{\left(\qquad '' \qquad\right)^{1/2} - k} \right|}$$

$$+ \operatorname{Im} \frac{1}{\frac{\hbar^2 k^2}{2m_c} + \Delta - \hbar\omega - \frac{\hbar^2 k^2}{2m_v} + i\frac{g_v^2 \hbar}{k} \ln\left|\frac{\left(\frac{2m_v}{\hbar^2}\left(\frac{\hbar^2 k^2}{2m_c} + \Delta - \hbar\omega + \hbar\omega_0\right)\right)^{1/2} + k}{\left(\quad '' \quad \right)^{1/2} - k}\right| + i\frac{g_c^2 \hbar}{k} \ln\left|\frac{\left(\frac{2m_c}{\hbar^2}\left(\hbar\omega_0 - \frac{\hbar^2 k^2}{2m_c}\right)\right)^{1/2} + k}{\left(\quad '' \quad \right)^{1/2} - k}\right| } \tag{5.2}$$

To perform these integrals we need to make use of the following;

$$\delta(f(x)) = \frac{1}{df/dx}\,\delta(x - x_0) \quad , \text{ where } f(x_0) = 0 \; .$$

Also the last two integrands can be rationalized. In the denominator of each we will then have the sum of the squares of the real part of the denominator and the imaginary part. The former is much greater than the latter for all values of k except where it goes to zero at

$$k = \left(\frac{2m_v}{\hbar^2}\left(\frac{\hbar^2 k^2}{2m_c} + \Delta - \hbar\omega + \hbar\omega_0\right)\right)^{1/2} .$$

Neglecting the smaller term will then cause unphysical behavior when the values of ω are such that this value of k is in the range of integration of k. This happens at

$$\hbar\omega = \Delta \qquad \text{and} \qquad \hbar\omega = \Delta - \frac{m_v - m_c}{m_c}\hbar\omega_0 \; .$$

These integrals will then have the form:

$$\int dx \, x \, \frac{\ln\left|\dfrac{(A+BX^2)^{1/2}+X}{(A+BX^2)^{1/2}-X}\right|}{(CX^2+D)^2} = \frac{-1}{2C} \, \frac{\ln\left|\dfrac{(A+BX^2)^{1/2}+X}{(A+BX^2)^{1/2}-X}\right|}{CX^2+D}$$

$$+ \, B/C\left(\frac{1}{BC-D(A-1)}\right)\left[\frac{C}{D\sqrt{B}} \, \frac{1}{(C/D-A/B)^{1/2}} \tan^{-1}\left(\frac{(C/D-A/B)^{1/2}X}{(1+A/B\,X^2)^{1/2}}\right)\right.$$

$$\left. - \, \frac{A-1}{B^{3/2}} \, \frac{1}{(-\frac{1}{B})^{1/2}} \tan^{-1}\left(\frac{(-\frac{1}{B})^{1/2}X}{(1+A/B\,X^2)^{1/2}}\right)\right] .$$

Considering the first term of (5.2) again, we need to know the zero of the function in the argument. To find it approximately, we expand the $\tan^{-1}$ terms around

$$k = \left(\frac{m_v m_c}{m_v - m_c} \, 2/\hbar^2 (\hbar\omega - \Delta)\right)^{1/2} ,$$

which is the zero of the algebraic part of the argument, and take only the first term. With these approximations, which take advantage of the smallness of g_v and g_c, we can evaluate all the integrals and get the absorption explicitly, but first we examine the form of Im G_r to see what the analysis says about the density of states. Only the delta-function term is non-zero below $E=\Delta+\hbar\omega_0$. If we neglect the $\tan^{-1}$ terms, we would have the density of states of the free particle,

$$\delta(E-\hbar^2k^2/2m_\ell-\Delta\delta_{\ell,c}+\mu)$$

and we would have reached the familiar result for the absorption that $\alpha\sim(\hbar\omega-\Delta)^{1/2}$

This tells us there are no states below $E=\Delta$ for $\ell=c$ and no absorption until $\hbar\omega=\Delta$, both of which we knew. But the $\tan^{-1}$ terms cause this edge to have a tail i.e. states below the edge, which is the fuzzing out we expected. As we shall see later, this allows absorption at energies less than $\hbar\omega=\Delta$. At $\hbar\omega=\Delta+\hbar\omega_0$ the other two terms in the expression for the absorption become non-zero. This is the energy at which real phonon emission is possible. Below this energy only virtual phonon states exist so the quasi-particle (dressed electron) is stable; above this energy the quasi-particle can decay, so that its lifetime is finite. In Green's function analysis this finite lifetime is associated with a complex self-energy which is just what appeared in our analysis, i.e. Σ went from a real to an imaginary quantity at $\hbar\omega=\Delta+\hbar\omega_0$. The reason something similar to this does not occur at multiple phonon emission energies, e.g. $\hbar\omega=\Delta+2\hbar\omega_0$, is that the diagrams we summed only contained one phonon intermediate states.

Carrying out the integrations one obtains for α:

$$\alpha = \frac{2e^2|V(k)|^2 4\pi^3}{c\,\epsilon^{1/2} m\omega \; \hbar^2\left(\frac{m_v - m_c}{m_v m_c}\right)} \left(\hbar\omega - \Delta + \frac{2g_c^2\hbar}{\left(\frac{2}{\hbar^2}\frac{m_c m_v}{m_v - m_c}(\hbar\omega - \Delta)\right)^{1/2}} \right.$$

$$\times \tan^{-1}\left(\frac{\left(-\frac{2m_c}{\hbar^2}\left(\frac{m_v}{m_v - m_c}(\hbar\omega-\Delta) - \hbar\omega_0\right)\right)^{1/2}}{\left(\frac{2}{\hbar^2}\frac{m_c m_v}{m_v - m_c}(\hbar\omega - \Delta)\right)^{1/2}} \right)$$

$$\left. + \frac{2g_v^2\hbar}{\left(\frac{2}{\hbar}\frac{m_c m_v}{m_v - m_c}(\hbar\omega - \Delta)\right)^{1/2}} \tan^{-1}\left(\frac{\left(-\frac{2m_v}{\hbar^2}\left(\frac{m_c}{m_v - m_c}(\hbar\omega-\Delta) + \hbar\omega_0\right)\right)^{1/2}}{\left(\frac{2}{\hbar^2}\frac{m_c m_v}{m_v - m_c}(\hbar\omega - \Delta)\right)^{1/2}} \right) \right)^{1/2}. \tag{5.3}$$

when $\hbar\omega < \Delta + \hbar\omega_0$

As stated this is real for values less than $\hbar\omega = \Delta$ because the $\tan^{-1}$ factors are positive and real quantities for $\hbar\omega < \Delta$.

For $2\hbar\omega_0 + \Delta > \hbar\omega > \hbar\omega_0 + \Delta$,

$$\alpha = \frac{2e^2|V(k)|^2 4\pi^2}{c\,\epsilon^{1/2} m\omega}\left[-g_v^2\hbar\left(-\frac{1}{\hbar\,\frac{m_c-m_v}{m_c m_v}}\right.\right.$$

$$\times\;\frac{\ln\left|\dfrac{\left(\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-2\hbar\omega_0)\right)^{\frac{1}{2}}+\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{\frac{1}{2}}}{\left(\qquad \text{''} \qquad\right)^{\frac{1}{2}}-\left(\qquad \text{''} \qquad\right)^{\frac{1}{2}}}\right|}{\left(\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)+\hbar\omega-\Delta\right)}$$

$$+\;\frac{\frac{2m_v\omega_0}{\hbar}}{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_v m_c}}\;\frac{1}{\frac{2m_v\omega_0}{\hbar}\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}+2(\hbar\omega-\Delta)}$$

$$\times\left\{\frac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}}{(\hbar\omega-\Delta)\left(\frac{2m_v\omega_0}{\hbar}\right)^{\frac{1}{2}}}\;\frac{1}{\left(\dfrac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_v m_c}}{\hbar\omega-\Delta}+\dfrac{\hbar}{2m_v\omega_0}\right)}\right.$$

$$\times \tan^{-1}\left(\frac{\left(\frac{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_v m_c}}{\hbar\omega - \Delta} + \frac{\hbar}{2 m_v \omega_0} \right)^{\frac{1}{2}} \left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right)^{\frac{1}{2}}}{\left(1 - \hbar/2m_v\omega_0 \left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right) \right)^{\frac{1}{2}}} \right)$$

$$+ \frac{2\hbar}{2m_v\omega_0 i} \tan^{-1}\left(\frac{i\left(\frac{\hbar}{2m_v\omega_0} \right)^{\frac{1}{2}} \left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right)^{\frac{1}{2}}}{\left(1 - \frac{\hbar}{2m_v\omega_0}\left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right) \right)^{\frac{1}{2}}} \right) \Bigg\}$$

$$+ g_c^2 \hbar \left(\frac{\frac{-m_c m_v}{\hbar^2(m_c - m_v)} \ln\left| \frac{\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \hbar\omega_0 - \Delta) \right)^{\frac{1}{2}} + \left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right)^{\frac{1}{2}}}{\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \hbar\omega_0 - \Delta) \right)^{\frac{1}{2}} - \left(-\frac{2m_v}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right)^{\frac{1}{2}}} \right|}{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0) \right) + \hbar\omega - \Delta} \right.$$

$$+ \frac{\frac{2m_c}{\hbar^2}(\hbar\omega - \hbar\omega_0 - \Delta)}{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}} \left(\frac{1}{\frac{2m_c}{\hbar^2}(\hbar\omega - \hbar\omega_0 - \Delta)\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v} - \left(\frac{m_c}{m_v} - 1 \right)(\hbar\omega - \Delta)} \right)$$

$$\left\{ \frac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}}{(\hbar\omega-\Delta)\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\hbar\omega_0-\Delta)\right)^{\frac{1}{2}}} \times \frac{1}{\left(\frac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}}{\hbar\omega-\Delta} - \frac{\frac{m_c}{m_v}-1}{\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)}\right)^{\frac{1}{2}}} \right.$$

$$\tan^{-1}\left(\frac{\left(\frac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_c m_v}}{\hbar\omega-\Delta} - \frac{\frac{m_c}{m_v}-1}{\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)}\right)^{\frac{1}{2}}\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{\frac{1}{2}}}{\left(1+\frac{m_c/m_v\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)}{\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)}\right)^{\frac{1}{2}}} \right)$$

$$\left. -\frac{\frac{m_c}{m_v}-1}{\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\, i} \tan^{-1}\left(\frac{\frac{i\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{\frac{1}{2}}}{\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{\frac{1}{2}}}}{\left(1+\frac{\frac{m_c}{m_v}\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)}{\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)}\right)^{\frac{1}{2}}} \right) \right\} \Bigg)$$

$$+ g_c^2 \hbar \left(- \frac{1}{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}} \ln \left| \frac{\left(-\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - 2\hbar\omega_0)\right)^{\frac{1}{2}} + \left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0)\right)^{\frac{1}{2}}}{\left(\quad '' \quad \right)^{\frac{1}{2}} - \left(\quad '' \quad \right)^{\frac{1}{2}}} \right| \right.$$

$$\frac{}{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0)\right) + \hbar\omega - \Delta}$$

$$+ \frac{\left(-2\frac{m_c\omega_0}{\hbar}\right)}{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}} \left(\frac{1}{-2\frac{m_c\omega_0}{\hbar}\frac{\hbar^2}{2}\frac{m_c - m_v}{m_v m_c}} \right) \left\{ \frac{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}}{(\hbar\omega - \Delta)\left(-2\frac{m_c\omega_0}{\hbar}\right)^{\frac{1}{2}}} \right.$$

$$\frac{1}{\left(\frac{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}}{\hbar\omega - \Delta} + \frac{\hbar}{2m_c\omega_0}\right)^{\frac{1}{2}}} \tan^{-1}\left(\frac{\left(\frac{\frac{\hbar^2}{2}\frac{m_c - m_v}{m_c m_v}}{\hbar\omega - \Delta} + \frac{\hbar}{2m_c\omega_0}\right)^{\frac{1}{2}}\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0)\right)^{\frac{1}{2}}}{\left(1 + \frac{\hbar}{2m_c\omega_0}\left(\frac{2m_c}{\hbar^2}(\hbar\omega - \Delta - \hbar\omega_0)\right)\right)^{\frac{1}{2}}} \right) \Bigg\} \Bigg)$$

$$-g_v^2\hbar\left(\frac{-\dfrac{1}{\hbar^2\dfrac{m_c-m_v}{m_cm_v}} \ln\left|\dfrac{\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-2\hbar\omega_0)\right)^{1/2}+\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}}{\left(\quad ''\quad\right)^{1/2}-\left(\quad ''\quad\right)^{1/2}}\right|}{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_cm_v}\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)+\hbar\omega-\Delta}\right.$$

$$+\frac{\frac{2m_v}{\hbar^2}(\hbar\omega_0+\Delta-\hbar\omega_0)}{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_cm_v}} \times \frac{1}{\left(\frac{2m_v}{\hbar^2}(\hbar\omega_0+\Delta-\hbar\omega)\right)\frac{\hbar^2}{2}\frac{m_c-m_v}{m_vm_c}-(\hbar\omega-\Delta)\left(\frac{m_v}{m_c}-1\right)}$$

$$\left\{\frac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_cm_v}}{(\hbar\omega-\Delta)\left(\frac{2m_v}{\hbar^2}(\hbar\omega_0+\Delta-\hbar\omega)\right)}\times\frac{1}{\left(\dfrac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_vm_c}}{\hbar\omega-\Delta}-\dfrac{\frac{m_v}{m_c}-1}{\left(\frac{2m_v}{\hbar^2}(\hbar\omega_0+\Delta-\hbar\omega)\right)}\right)^{1/2}}\right.$$

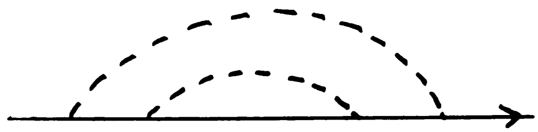
$$\tan^{-1}\left(\frac{\left(\dfrac{\frac{\hbar^2}{2}\frac{m_c-m_v}{m_cm_v}}{\hbar\omega-\Delta}-\dfrac{\frac{m_v}{m_c}-1}{\frac{2m_v}{\hbar^2}(\hbar\omega_0+\Delta-\hbar\omega)}\right)^{1/2}\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}}{\left(1+\left(\frac{m_v}{m_c}-1\right)\Big/\left(-\frac{2m_v}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)\right)\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{1/2}}\right)$$

$$\frac{-\frac{m_v}{m_c}-1}{i\left(\frac{2m_v}{\hbar^2}(\Delta+\hbar\omega_0-\hbar\omega)\right)}\tan^{-1}\left(\frac{\dfrac{i\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)^{\frac{1}{2}}}{\left(\frac{2m_v}{\hbar^2}(\Delta+\hbar\omega_0-\hbar\omega)\right)^{\frac{1}{2}}}}{\left(1+\dfrac{\frac{m_v}{m_c}-1}{\left(\frac{2m_c}{\hbar^2}(\hbar\omega-\Delta-\hbar\omega_0)\right)\Big/\frac{2m_v}{\hbar^2}(\Delta+\hbar\omega_0-\hbar\omega)}\right)^{\frac{1}{2}}}\right)\Bigg\}\Bigg)$$

$$+\ (5.3) \tag{5.4}$$

VI. A Two-Phonon Diagram Correction

Our previous results for the inter-band absorption have been derived using an approximation in which processes having more than one phonon "dressing" the electron at one time are not included. These processes should affect the self-energy of the polaron and show structure at multiples of phonon energies above the band-edge because of the possibility of real multiple phonon emission at those energies. To investigate the way multiple phonon processes affect the absorption calculation and results we will calculate the Green's function for a two-phonon process as an example. The process corresponds to the following diagram:



According to the Feynman rules, the self-energy corresponding to this diagram is

$$\Sigma = \frac{g^4 \hbar^3}{(2\pi)^8}\int \frac{d^3p_1\, d^3p_2\, d\omega_1\, d\omega_2}{|p-p_1|^2\,|p_1-p_2|^2}\; \frac{\omega_0^2\left(\frac{1}{\omega_0+i(\omega-\omega_1)}+\frac{1}{\omega_0-i(\omega-\omega_1)}\right)}{\left(i\hbar\omega_1-\frac{\hbar^2p^2}{2m_\ell}-\Delta\delta_{\ell,c}+\mu\right)^2}$$

$$\times\frac{\left(\frac{1}{\omega_0+i(\omega_1-\omega_2)}+\frac{1}{\omega_0+i(\omega_1-\omega_2)}\right)}{i\hbar\omega_2-\frac{\hbar^2p_2^2}{2m_\ell}-\Delta\delta_{\ell,c}+\mu}\;.$$

The poles in the complex ω_2-plane are at $\pm i\omega_0+\omega_1$ and

$$\omega_2=\frac{1}{\hbar}\left(i\mu-i\hbar^2p_2^2/2m_\ell-i\Delta\,\delta_{\ell,c}\right)$$

The last pole is in the lower half plane for ℓ=c and the upper half plane for ℓ=v. If we close the contour in the upper half plane for ℓ=c and in the lower for ℓ=v, the result of the integration is:

$$\Sigma \sim \int \frac{d^3p_1\, d^3p_2\, d\omega_1 \left(\frac{1}{\omega_0+i(\omega-\omega_1)}+\frac{1}{\omega_0-i(\omega-\omega_1)}\right)2\pi\omega_0^2}{|p-p_1|^2\,|p_1-p_2|^2\left(i\hbar\omega_1-\frac{\hbar^2p_1^2}{2m_\ell}-\Delta\delta_{\ell,c}+\mu\right)^2\left(\mp i\hbar\omega_0+i\hbar\omega_1-\frac{\hbar^2p^2}{2m_\ell}-\Delta\right)}$$

$$\overline{\times\left(i\hbar\omega_1\mp\hbar\omega_0-\frac{\hbar^2p_2^2}{2m_\ell}-\Delta\delta_{\ell,c}+\mu\right)}\;,$$

(upper sign is for ℓ=c, lower for ℓ=v). The poles in the ω_1-plane are at $\omega_1 = \omega \pm i\omega_0$, $\frac{1}{\hbar}(\mp i\hbar\omega_0 - i\frac{\hbar^2 p_2^2}{2m\ell} - i\Delta\delta_{\ell,c} + i\mu)$, $\frac{1}{\hbar}(-i\hbar^2 p_2^2/2m_\ell - i\Delta\delta_{\ell,c} + i\mu)$.

The last two poles are in the lower half ω_1-plane if ℓ=c, and the upper for ℓ=v. Once again we close the contour in the upper half-plane for ℓ=c, and the lower half-plane for ℓ=v. The result of the ω_1 integration is:

$$\Sigma \sim (2\pi)^2 \int \frac{d^3p_1\, d^3p_2\, \omega_0^2}{|p-p_1|^2 |p_1-p_2|^2 \left(i\hbar\omega \mp \hbar\omega_0 - \frac{\hbar^2 p_1^2}{2m_\ell} - \Delta\delta_{\ell,c} + \mu\right)^2 \times}$$

$$\overline{\times\left(\mp\hbar\omega_0 \mp \hbar\omega_0 + i\hbar\omega - \hbar^2 p_2^2/2m_\ell - \Delta\delta_{\ell,c} + \mu\right)}$$

Going over to spherical coordinates and taking the polar axis to lie along the $\vec{p}_1$ direction for the $\vec{p}_2$ integration and along $\vec{p}$ for the $\vec{p}_1$ integration we see that the above becomes:

$$\Sigma \sim (2\pi)^2 \omega_0^2 \int \frac{p_1^2 p_2^2\, dp_1\, dp_2 \sin\theta_1 \sin\theta_2\, d\theta_1\, d\theta_2}{(p^2 + p_1^2 - 2pp_1\cos\theta_1)(p_1^2 + p_2^2 - 2p_1p_2\cos\theta_2) \times}$$

$$\overline{\times\left(i\hbar\omega \mp \hbar\omega_0 - \frac{\hbar^2 p^2}{2m_\ell} - \Delta\delta_{\ell,c} + \mu\right)^2 \left(i\hbar\omega \mp 2\hbar\omega_0 - \frac{\hbar^2 p_2^2}{2m_\ell} - \Delta\delta_{\ell,c} + \mu\right)}$$

$$= \frac{(2\pi)^4 \omega_0^2}{4p} \int \frac{dp_1\, dp_2\, p_2 \ln|p_1^2 + p^2 - 2pp_1\cos\theta_1|}{\left(i\hbar\omega \mp \hbar\omega_0 - \frac{\hbar^2 p_1^2}{2m_e} - \Delta\delta_{l,c} + \mu\right)^2}$$

$$\times \left. \frac{\ln|p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta_2|}{\left(i\hbar\omega \mp 2\hbar\omega_0 - \frac{\hbar^2 p_2^2}{2m_e} - \Delta\delta_{l,c} + \mu\right)} \right|_0^{\pi}$$

$$= \frac{(2\pi)^4 \omega_0^2}{16p} \int \frac{dp_1\, dp_2 \ln\left|\frac{p_1+p_2}{p_1-p_2}\right| \ln\left|\frac{p+p_1}{p-p_1}\right|}{\left(i\hbar\omega \mp \hbar\omega_0 - \frac{\hbar^2 p_1^2}{2m_e} - \Delta\delta_{l,c} + \mu\right)^2 \left(i\hbar\omega \mp 2\hbar\omega_0 - \frac{\hbar^2 p_2^2}{2m_e} - \Delta\delta_{l,c} + \mu\right)} .$$

The p_2 integration has the form

$$\int_0^{\infty} \frac{dx\; x \ln\left|\frac{P_1+x}{P_1-x}\right|}{(B - cx^2)} .$$

It is even in x so we can write it as:

$$-\frac{1}{2c} \int_{-\infty}^{\infty} dx \; \frac{x\left(\ln|x+P_1| - \ln|x-P_1|\right)}{\left(x - \sqrt{B/c}\right)\left(x + \sqrt{B/c}\right)} .$$

The integrand vanishes at infinity sufficiently fast so that the integral along an arc at infinity gives no contribution, hence the integral equals the contour integral

$$-\frac{1}{2C}\int_{A} dx\; \frac{x\left(\ln|x+p_1|-\ln|x-p_1|\right)}{\left(x-\sqrt{B/C}\right)\left(x+\sqrt{B/C}\right)},$$

where A is

The pole enclosed is at $x=(B/C)^{1/2}$, so the value of the integral is

$$\frac{-\pi i}{2C}\left(\ln\left|\sqrt{B/C}+p_1\right|-\ln\left|\sqrt{B/C}-p_1\right|\right)$$

Thus

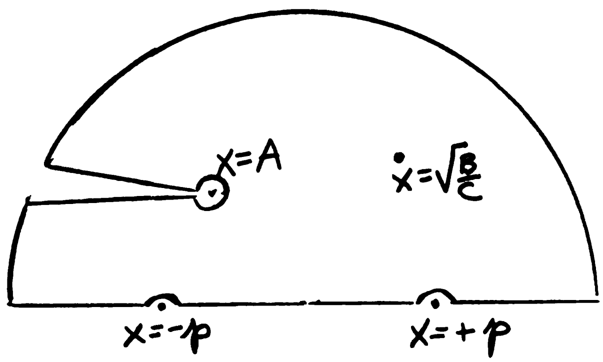
$$\Sigma \sim \int_0^\infty \frac{\pi^5 \omega_0^2 m_e i}{2p\hbar^2}\ln\left|\frac{\left(\frac{2m_e}{\hbar^2}(i\hbar\omega\mp 2\hbar\omega_0-\Delta\delta_{e,c}+\mu)\right)^{\frac{1}{2}}+p_1}{\left(\quad '' \quad\right)^{\frac{1}{2}}-p_1}\right|$$

$$\times\left(\ln\left|\frac{p_1+p}{p_1-p}\right|\Big/\left(i\hbar\omega\mp\hbar\omega_0-\frac{\hbar^2 p_1^2}{2m_e}-\Delta\delta_{e,c}+\mu\right)^2\right)dp_1$$

This integrand is also even so it is of the form

$$\frac{1}{2C^2}\int_{-\infty}^{\infty} dx\,\frac{(\ln|A+x|-\ln|A-x|)(\ln|p+x|-\ln|p-x|)}{(x^2-B/C)^2}\ .$$

Here the poles are at $x=\pm A$, $\pm p$, $\pm(B/C)^{1/2}$. We use the following contour to avoid all singularities except the one at $x=(B/C)^{1/2}$:



Then

$$\int_\Gamma dx\,\frac{(\ln|A+x|-\ln|A-x|)(\ln|p+x|-\ln|p-x|)}{(x^2-B/C)^2}$$

$$=\frac{1}{2B^2}\int_\Gamma dx\,(\ln|A+x|-\ln|A-x|)(\ln|p+x|-\ln|p-x|)$$

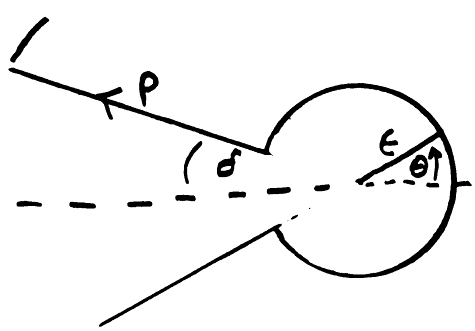
$$\times\left(\frac{1}{(x-\sqrt{B/C})^2}+\frac{1}{(x+\sqrt{B/C})^2}-\frac{2}{(x^2-B/C)}\right)$$

$$= \frac{2\pi i}{(2B)^2}\Bigg[\left(\ln\left|A+\sqrt{B/c}\right| - \ln\left|A-\sqrt{B/c}\right|\right)\left(\frac{1}{p+\sqrt{B/c}}+\frac{1}{p-\sqrt{B/c}}\right)$$

$$+\left(\frac{1}{A+\sqrt{B/c}}+\frac{1}{A-\sqrt{B/c}}\right)\left(\ln\left|p+\sqrt{B/c}\right| - \ln\left|p-\sqrt{B/c}\right|\right)$$

$$-\frac{\left(\ln\left|A+\sqrt{B/c}\right| - \ln\left|A-\sqrt{B/c}\right|\right)\left(\ln\left|p+\sqrt{B/c}\right| - \ln\left|p-\sqrt{B/c}\right|\right)}{\sqrt{B/c}}\Bigg].$$

Since the integral along the semi-circular part of the contour is zero, the only difference between the integral over this contour and the integral from $-\infty$ to ∞ is the key-hole-like part that avoids the branch cut of the log function, so we must subtract its contribution.



$$\int_{\infty}^{\epsilon} (\ln \rho + i(\pi-\delta))\Big(\ln|p + A + \rho e^{i(\pi-\delta)}|$$

$$-\ln|p - A - \rho e^{i(\pi-\delta)}|\Big)\frac{1}{(2B)^2}\Bigg(\frac{1}{(A+\rho e^{i(\pi-\delta)} - \sqrt{B/C})^2}$$

$$+\frac{1}{(A+\rho e^{i(\pi-\delta)} + \sqrt{B/C})^2} - \frac{2}{(A+\rho e^{i(\pi-\delta)})^2 - B/C}\Bigg) e^{i(\pi-\delta)}\, d\rho$$

$$-\int_{\epsilon}^{\infty} (\ln \rho + i(\pi-\delta))\Big(\ln|p + A + \rho e^{i(\delta-\pi)}|$$

$$-\ln|p - A - \rho e^{i(\delta-\pi)}|\Big)\frac{1}{(2B)^2}\Bigg(\frac{1}{(A+\rho e^{i(\delta-\pi)} - \sqrt{B/C})^2}$$

$$+\frac{1}{(A+\rho e^{i(\delta-\pi)} + \sqrt{B/C})^2} - \frac{2}{(A+\rho e^{i(\delta-\pi)})^2 - B/C}\Bigg)$$

$$-\int_{\delta-\pi}^{\pi-\delta} i\epsilon e^{i\theta} d\theta \left(\ln\epsilon + i\theta\right)\left(\ln|p+A+\epsilon e^{i\theta}| - \ln|\right.$$

$$\left. - \ln|p-A-\epsilon e^{i\theta}|\right).$$

The last term goes to zero as $\epsilon \to 0$, and the first two add up to:

$$2\pi i \int_{\epsilon}^{\infty} \frac{d\rho}{(2B)^2} \left(\ln|p+A-\rho| - \ln|p-A+\rho|\right)\left(\frac{1}{(A-\rho-\sqrt{B/c})^2}\right.$$

$$\left. + \frac{1}{(A-\rho+\sqrt{B/c})^2} - \left(\frac{1}{A-\rho-\sqrt{B/c}} - \frac{1}{A-\rho+\sqrt{B/c}}\right)\sqrt{\frac{c}{B}}\right)$$

$$= \frac{2\pi i}{(2B)^2}\Bigg[\left(\ln|p+A-\rho| - \ln|p-A+\rho|\right)\left(\frac{1}{A-\rho-\sqrt{B/c}}\right.$$

$$\left. + \frac{1}{A-\rho-\sqrt{B/c}}\right)\Bigg|_{\epsilon}^{\infty} + \int_{\epsilon}^{\infty} d\rho \left(\frac{1}{p+A-\rho} + \frac{1}{p-A+\rho}\right)$$

$$\left(\frac{1}{A-\rho-\sqrt{B/C}}+\frac{1}{A-\rho+\sqrt{B/C}}\right)-\sqrt{C/B}\int_{\epsilon}^{\infty}\Big(\ln|p+A-\rho|$$

$$-\ln|p-A+\rho|\Big)\left(\frac{1}{A-\rho-\sqrt{B/C}}-\frac{1}{A-\rho+\sqrt{B/C}}\right)\Bigg]$$

$$=\frac{2\pi i}{(2B)^2}\Bigg[\ln\left|\frac{p+A}{p-A}\right|\left(\frac{1}{A-\sqrt{B/C}}+\frac{1}{A+\sqrt{B/C}}\right)+\frac{\ln\left|\frac{A-\sqrt{B/C}}{A+p}\right|}{\sqrt{B/C}+p}$$

$$+\frac{\ln\left|\frac{A+\sqrt{B/C}}{p+A}\right|}{p-\sqrt{B/C}}+\frac{\ln\left|\frac{A-p}{A-\sqrt{B/C}}\right|}{\sqrt{B/C}-p}+\frac{\ln\left|\frac{A-p}{A+\sqrt{B/C}}\right|}{-p-\sqrt{B/C}}$$

$$-\sqrt{C/B}\int_{\epsilon}^{\infty}d\rho\Big(\frac{\ln|p+A-\rho|}{A-\rho-\sqrt{B/C}}+\frac{\ln|p-A+\rho|}{A+\sqrt{B/C}-\rho}$$

$$-\frac{\ln|p+A-\rho|}{A+\sqrt{B/C}-\rho}-\frac{\ln|p-A+\rho|}{A-\sqrt{B/C}-\rho}\Big)\Bigg]\;.$$

The last four integrals look deceptively simple, however, there appears to be no anti-derivative involving only elementary functions for this type of integral. What we can do is to expand ln(p+x) through the linear term in p; then we can integrate, but our answer is good only for small p (the polaron momentum). The integrals become:

$$\int_{\epsilon}^{\infty} \left(\frac{2p}{(A-\rho)(A-\sqrt{B/C}-\rho)} - \frac{2p}{(A-\rho)(A+\sqrt{B/C}-\rho)} \right) d\rho$$

$$= 2p\left(\frac{\ln|A-\rho|\,\ln|A-\sqrt{B/C}-\rho|}{\sqrt{B/C}} + \frac{\ln|A-\rho|\,\ln|A+\sqrt{B/C}-\rho|}{\sqrt{B/C}} \right)\Bigg|_{\epsilon}^{\infty}$$

$$= \frac{2p}{\sqrt{B/C}}\left(\ln A \,\ln|A-\sqrt{B/C}| + \ln A\,\ln|A+\sqrt{B/C}| \right)$$

So the total contribution from the key-hole part of the contour is:

$$\frac{2\pi i}{(2B)^2}\left[\ln\left|\frac{p+A}{p-A}\right| \left(\frac{2A}{A^2-B/C}\right) + \frac{\ln\left|\frac{A^2-B/C}{A^2-p^2}\right|}{\sqrt{B/C}+p} + \frac{\ln\left|\frac{A^2-B/C}{A^2-p^2}\right|}{p-\sqrt{B/C}} \right.$$

$$+\frac{C}{B}\, 2p \ln|A| \ln\left|A^2-B/C\right|\Big] \; .$$

Then

$$\frac{1}{2c^2}\int_{-\infty}^{\infty} dx \frac{(\ln|A+x|-\ln|A-x|)(\ln|p+x|-\ln|p-x|)}{(x^2-B/C)^2}$$

$$=\frac{2\pi i}{8C^2B^2}\Big[\ln\left|\frac{A+\sqrt{B/C}}{A-\sqrt{B/C}}\right|\frac{2p}{p^2-\frac{B}{C}}+\frac{2A}{A^2-B/C}\ln\left|\frac{p+\sqrt{B/C}}{p-\sqrt{B/C}}\right|$$

$$-\ln\left|\frac{A+\sqrt{B/C}}{A-\sqrt{B/C}}\right|\ln\left|\frac{p+\sqrt{B/C}}{p-\sqrt{B/C}}\right|\sqrt{\frac{C}{B}}-\ln\left|\frac{p+A}{p-A}\right|\left(\frac{2A}{A^2-B/C}\right)$$

$$-\ln\left|\frac{A^2-B/C}{A^2-p^2}\right|\frac{2p}{p^2-B/C}-\frac{C}{B}\,2p\ln|A|\ln\left|A^2-\frac{B}{C}\right|\Big]$$

where

$$A=\left(\frac{2m_\ell}{\hbar^2}(\hbar\omega\mp 2\hbar\omega_0-\Delta\delta_{\ell,c}+\mu)\right)^{1/2}$$

$$B = (\pm\hbar\omega_0 - \hbar\omega + \Delta\delta_{\ell,c} - \mu)\;,\; C = \frac{\hbar^2}{2m_\ell}\;.$$

Consider the term

$$\ln\left|\frac{A+\sqrt{B/C}}{A-\sqrt{B/C}}\right| = \ln\left|\frac{\left(\frac{2m_\ell}{\hbar^2}(\hbar\omega \mp 2\hbar\omega_0 - \Delta\delta_{\ell,c} + \mu)\right)^{\frac{1}{2}} +}{(\qquad ''\qquad)^{\frac{1}{2}} +}\right.$$

$$\left.\frac{+\left(\frac{2m_\ell}{\hbar^2}(\pm\hbar\omega_0 - \hbar\omega + \Delta\delta_{\ell,c} + \mu)\right)^{\frac{1}{2}}}{-(\qquad ''\qquad)^{\frac{1}{2}}}\right|\,,$$

we have a situation here similar to that which we found in the study of the one-phonon diagrams when $\hbar\omega \geq \Delta + \hbar\omega_0 - \mu$ i.e. the log function causes Σ to become complex above and real below that value. This indicates we have sucessfully taken account of the possibility of double phonon emission by the inclusion of our two-phonon diagram.

VII. Conclusion

What do the previously described calculations signify? Let us review the principal assumptions which went into the calculations we have described and the results to which they led.

It was assumed that the only interaction taking place in the system was between electrons and longitudinal optical-phonons and that the interaction was weak enough so that a perturbation calculation was possible. This means we neglected the effects of impurities, other types of phonons, and the coloumb interaction between electrons.

It was found that the absorption curve near the absorption edge has a parabolic component $(\hbar\omega-\Delta)^{1/2}$ (as is the case in a simple independent electron band model) with some complicated additive corrections which have the following characteristics. Below the band edge we find a tail region of absorption, equation (5.3), like an Urbach tail[16]. At energies of one and two phonons above the edge we find there should be an onset of structure, equations (5.4) and (6.1), such that the absorption curve has discontinuous derivatives corresponding to absorption due to creation of phonons. A calculation of the size of the effect gives a magnitude in the neighborhood of .01 inverse centimeters for a material like InSb at an energy of $\Delta+\frac{3}{2}\hbar\omega_0$. This is near the limits of resolution, although at that energy the parabolic part has a magnitude of 2 inverse centimeters. The physical arguments presented make these features appear plausible, and the set of one phonon diagrams should give us a very accurate description of the structure between $\Delta+\hbar\omega_0$ and $\Delta+2\hbar\omega_0$ since we have included every process that could give an imaginary Σ in this range of energies.

There are reports in the literature of experimental findings that support our results. Structure has been found at longitudinal optical phonon energy intervals above the band edge energy in photoconductivity[17,18] and radiative recombination[19] measurements. Such structure has also been reported in actual absorption spectra by Ascarelli[20] and Larsen and Johnson[21]. The former found it in AgBr and the latter in InSb.

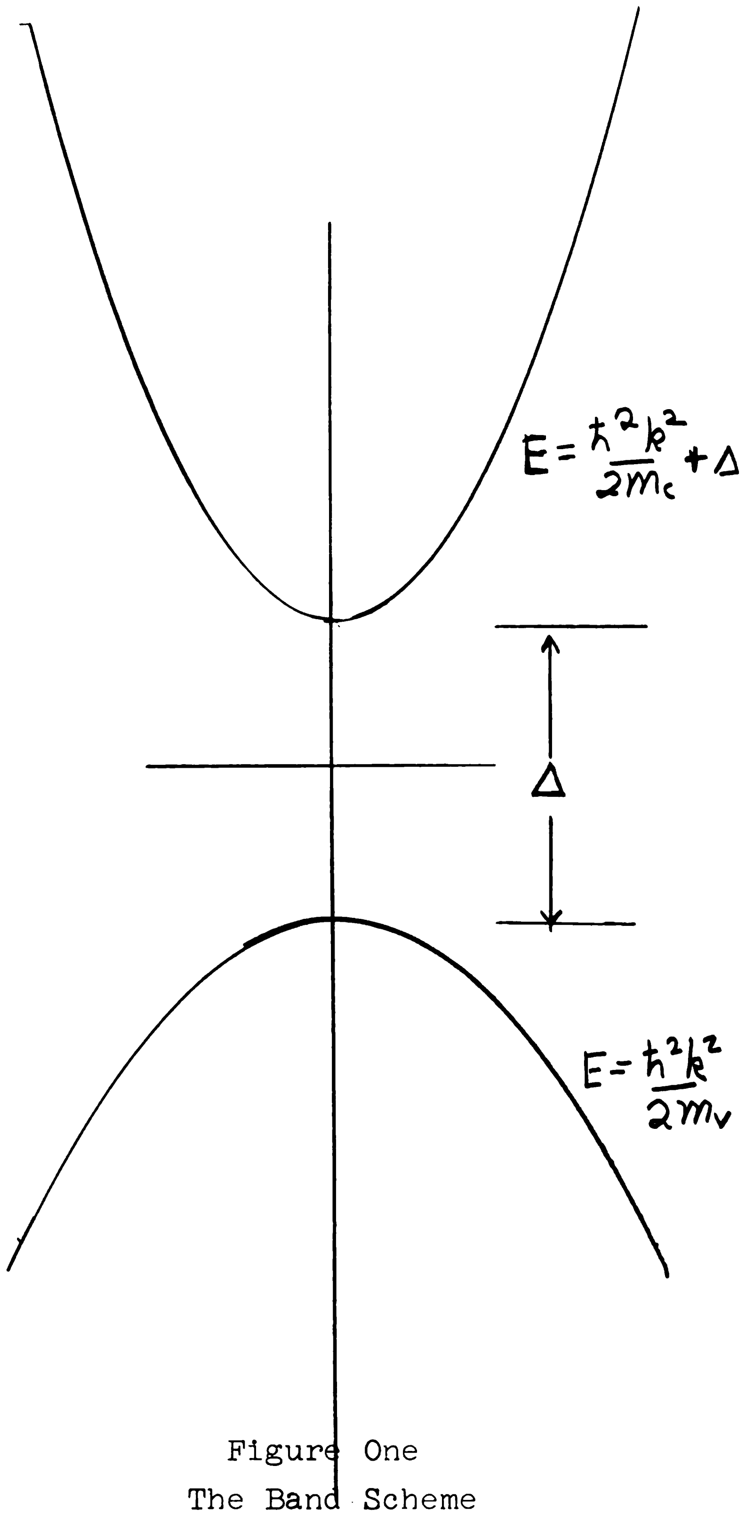


Figure One
The Band Scheme

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