GROUND STATE PERTURBATION THEORY FOR THE MANY ELECTRON SYSTEM IN A STATIC LATTICE: SOME PLASMON PROPERTIES OF INSULATORS

by

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I. INTRODUCTION

1. Background

The many-body problem of solid state physics can be treated in a unified fashion by employing the field-theoretic techniques of Feynman, Dyson, Schwinger, et al. These techniques, which allow the summation of an infinite number of terms in the perturbation series for quantities of interest, yield in a natural way both the "single-particle like" and the "collective" behavior of the system under consideration.

The homogeneous electron gas (i.e., a gas of interacting electrons in a uniform positively charged background) has been treated by these techniques by many authors (e.g., Schultz). In this thesis, a treatment of the zero-temperature inhomogeneous electron gas (specifically a gas of interacting electrons in the external field of a positively charged lattice) rather closely parallel to that of Schultz[1] for the homogeneous gas is reported along with an application of the theory. In particular, the energy and lifetime of the simplest excited state which derives from the collective behavior of the system (the single-plasmon state) will be calculated for certain simple insulator models.

2. Review

The homogeneous gas has been well studied and results are available in many textbooks and review articles. The first attempt at simultaneous extraction of the single particle and collective behavior of the electron gas (Bardeen and Pines) was, upon application of the

Random Phase Approximation (RPA), partially successful. Gell-Mann and Brueckner performed an explicit summation of the perturbation series and verified the correctness of RPA in the high density limit.

The following is a brief summary of some relevant work which has dealt with the inhomogeneous electron gas problem. Hubbard[2,3,4] gives the ground state energy in terms of the eigenvalues of a homogeneous integral equation for the "exact interaction." Wiser,[5,6] using the self-consistent-field (SCF) method of Ehrenreich and Cohen,[7,8] studies local field effects and calculates correlation and exchange contributions to the ground state energy. Using the results of Martin and Schwinger[9], Falk[10] studies the "dielectric matrix" in a Hartree-Fock approximation. [Luttinger[11] (at finite temperature) demonstrates that band theory is obtained from the single-particle propagator.] Frolich and Pelzer[12] show the relation between the dielectric constant and energy loss experiments. Pines[13], utilizing experimental oscillator strengths, makes crude estimates of certain optical properties of real solids. In particular, rough values of the plasmon energy and lifetime are given. Davies[14] finds approximate expressions for the single-particle lifetimes including certain local field effects at finite temperature. Penn[15] and Fry[16], using non-trivial values for the Bloch matrix elements, calculate numerically the zero frequency dielectric constant for semiconductors and insulators. Finally, Hubbard[17] gives simple results for the dielectric tensor which are subsequently improved by Adler[18,19].

3. Present Problem

The present work proceeds along the lines laid out by Schultz[1] and by DuBois[20,21]. First, we give a brief description of that portion of the general theory which is applicable. Since collective behavior can occur only if the particles of the system interact, there is no analog of the plasmon excited state in a non-interacting system. In other words, there is no excited eigenstate of the non-interacting system whose adiabatic transform is the plasmon excited state. So, following DuBois, some linear combination of such excited eigenstates is now sought. The most obvious choice is that one which results from operation on the unperturbed ground state by the density fluctuation operator. The amplitude of the Schrodinger state which results upon adiabatic transformation of this state so constructed is shown to be essentially the polarization propagator. The plasmon energy and lifetime is then defined so as to produce the correct time dependence for this approximate eigenstate of the system.

In order to perform some relevant numerical calculations, a simple band model used by Fry[16] which is representative of several real insulators is chosen. The wave function of the single conduction band is taken to be a plane wave orthogonalized to three isotropic valence bands which are represented by tight-binding wave functions. The resultant matrix elements are given by Fry[16].

II. GROUND STATE PERTURBATION THEORY FOR THE MANY ELECTRON SYSTEM IN A STATIC LATTICE: THE FORMALISM

1. The x-space Results

The problem under consideration is an electron gas interacting via coulomb interaction with positive charges in a static lattice. The system, static lattice plus electron gas, is electrically neutral and its hamiltonian is taken to be

$$H = \sum_{i=1}^{N} \left[\frac{pi^2}{2m} + V(\vec{r}_i)\right] + \frac{1}{2} \sum_{i=1}^{N} {}' \sum_{j=1} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \tag{1}$$

where the prime on the summation means exclude those terms where $i = j$, and $V(r_i)$ is the potential due to the static lattice. This hamiltonian is now cast into its second quantized form

$$H = \int d^3r \psi^+(\vec{r}) H_0'(r) \psi(\vec{r}) + \frac{1}{2} \int d^3r \int d^3r' \psi^+(\vec{r}) \psi^+(\vec{r}') v(\vec{r}-\vec{r}') \psi(\vec{r}') \psi(\vec{r})$$

$$= H_0' + H_1' \tag{2}$$

where

$$H_0'(r) = -\frac{\hbar^2 \nabla_{\vec{r}}^2}{2m} + V(\vec{r}) \tag{3a}$$

has eigen-solutions satisfying

$$H_0'(\vec{r}) \phi_{n\vec{k}}(\vec{r}) = \varepsilon_{n\vec{k}} \phi_{n\vec{k}}(\vec{r}) \quad , \tag{3b}$$

and

$$\psi(\vec{r}) = \sum_{n,\vec{k}} C_{n\vec{k}} \phi_{n\vec{k}}(\vec{r}) \tag{3c}$$

$$[C^+_{n\vec{k}}, C_{n'\vec{k}'}] = \delta_{nn'} \cdot \delta_{\vec{k}\vec{k}'}$$

$C^{+}_{n\vec{k}}$ and $C_{n\vec{k}}$ being the usual creation and destruction operators for a state of reduced wave vector $\vec{k}$ and band n. Also,

$$v(\vec{r} - \vec{r}') = \frac{e^2}{|\vec{r} - \vec{r}'|} \quad . \tag{4}$$

We make the following observations (hereafter usually dropping vector signs on space-coordinate arguments for ease of notation):

(1) H'_1 may be rearranged as follows:

$$H'_1 = \frac{1}{2}\int d^3r \int d^3r' \psi^{+}(r)\psi^{+}(r')\, v(r - r')\psi(r')\psi(r) \tag{5}$$

$$= \frac{1}{2}\int d^3r \int d^3r' \psi^{+}(r)\psi(r)\, v(r - r')\psi^{+}(r')\psi(r') - \frac{1}{2} Nv(0)$$

where $-\frac{1}{2} Nv(0)$ is called the "infinite self-energy".

(2) A one-body potential W may be added to and subtracted from the model hamiltonian as follows:

$$H = H'_0 + H'_1 = (H'_0 + W) + (H'_1 - W)$$

$$\equiv H_0 + H_1 \quad ,$$

where

$$W = \sum_{i=1}^{N} w(r_i) \tag{6}$$

and w(r) may be chosen for convenience. Note that now the one particle basis functions are solutions of this modified H_0 and the creation and destruction operators refer to the modified Bloch states. Also, the perturbation term H_1 contains both one- and two-body operators. Explicitly, we now write

$$H_0 = \int d^3r\psi^+(r)[-\frac{\hbar^2\nabla^2}{2m} + V(r) + w(r)]\psi(r) - \frac{1}{2}NV(0) \qquad (7a)$$

$$H_1 =$$

$$-\int d^3r\psi^+(r)w(r)\psi(r) + \frac{1}{2}\int d^3r\int d^3r\psi^+(r)\psi(r)V(r-r')\psi^+(r')\psi(r') \qquad (7b)$$

The n particle Green function defined in the Heisenberg picture by

$$G(x_1,..,x_n;x_1',..,x_n') \equiv (-i)^n<\Psi_o|T(\psi(x_1)...\psi(x_n)\psi^+(x_n')...\psi^+(x_1')|\Psi_o> \qquad (8a)$$

where $x = (r,t)$ and $|\Psi_o>$ is the exact ground state, can be analyzed using Wick's theorem[1] and the result is the well-known linked - cluster expansion:

$$G(x_1,...,x_n;x_1',...,x_n') =$$

$$= (-i)^n<\Phi_o|T(\psi(x_1)...\psi(x_n)\psi^+(x_n')...\psi^+(x_1')S)|\Phi_o>_{conn.} \qquad (8b)$$

Here, $|\Phi_o>$ is the ground state of the unperturbed system and the subscript "conn." means the series contains only "completely connected" terms. S is the usual S-matrix in the interaction picture and the field operators are also interaction picture operators:

$$S = 1 + \sum_{j=1}^{\infty}\frac{1}{j!}(-\frac{i}{\hbar})^j\int_{-\infty}^{\infty}dt_1\ldots\int_{-\infty}^{\infty}dt_jT(H_1(t_1)...H_1(t_j)) \quad , \qquad (9)$$

with T the Dyson time-ordering operator. The many particle Green function thus becomes a sum of terms whose factors involve the one- and two-body interactions and single particle Green functions G_o for the unperturbed system. Each term in the sum implicit in eq. (8b) is associated with a diagram constructed as follows:

(1) For an n-particle Green function, draw 2 n external points labeled by $x_1', \ldots, x_n'$ and $x_1, \ldots, x_n$

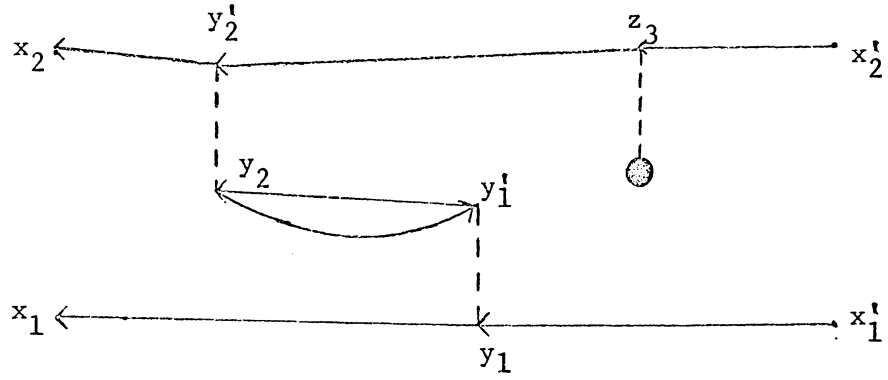
(2) For a term arising from the ℓth order in the expansion, that is, having k factors of $v(y-y')$ and $\ell - k$ factors of $w(z)$: draw k pairs of points labeled by $y_1, y_1'; \ldots; y_k, y_k'$ and $\ell - k$ points labeled by $z_{k+1}, z_{k+2}, \ldots, z_\ell$, connect each pair y_i, y_i' with a dotted line, and connect each z_j to a shaded circle with a dotted line.

(3) Connect all points with directed solid lines so that each external point x_i' has a line directed away from it, each internal point y_i, y_i' or z_i' has one line toward and one line directed away from it, and each external x_i has a line directed toward it.

(4) Every internal point must be connected to at least one pair of external points x_i, x_j' by solid or dotted lines; i.e., a diagram may not have disconnected parts.

An example of a diagram:

two particle Green function, third order term:



To write down the term in the series associated with a diagram,

(a) for each element $u_a \leftarrow\text{-------}\ u_b$ write $i\,G_o(u_a,u_b)$, where $G_o(u_a,u_b)$ is the unperturbed one-particle Green function:

$$G_o(u_a,u_b) = -i\langle\Phi_o|T(\psi(u_a)\psi^+(u_b))|\Phi_o\rangle \quad ;$$

(b) for each element y_i' --------- y_i write

$$-\frac{i}{\hbar}\,v(y_i' - y_i) \quad ;$$

(c) for each element z_i --------● write

$$-\frac{i}{\hbar}\,w(z_i) \quad ;$$

(d) write a (-1) factor for

(i) each closed loop of solid lines

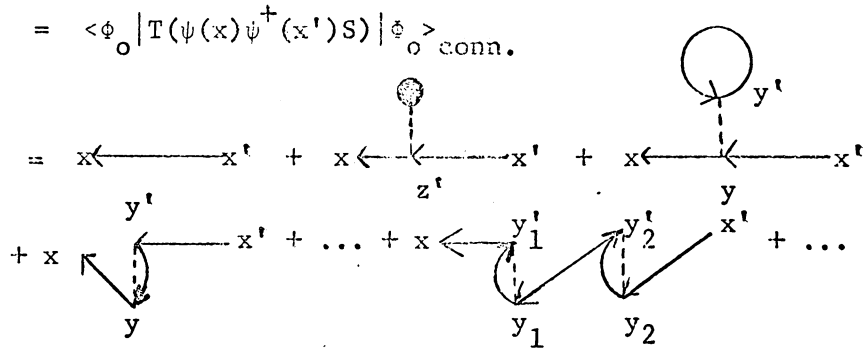
(ii) each "crossing" of one external solid line by another external solid line;

(e) integrate over all internal (i.e., y_i, y_i', z_i) variables from $-\infty$ to $+\infty$.

To get all the terms of a given order in the series, draw only those diagrams which are distinct. Diagrams which differ only through an interchange of a pair of y_i's are not distinct as this corresponds to merely a change of integration variables.

With the above results, integral equations for various important functions may be found. These integral equations incorporate sums of certain classes of terms in the perturbation series for either the S matrix or a Green function. Consider first the one-particle Green function expressed in diagrams according to the above rules:

$$i\,G(x,x') = \langle\phi_o|T(\psi(x)\psi^+(x')S)|\phi_o\rangle_{conn.}$$



$$= i\,G_o(x,x') + \int d^4z'\,iG_o(z',x')\left(\frac{-i}{\hbar}w(z')\right)iG_o(x,z')$$

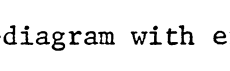
$$+ \int d^4y d^4y'\,iG_o(y,x')\left(\frac{-i}{\hbar}v(y'-y)\right)iG_o(y',y')iG_o(x,y)$$

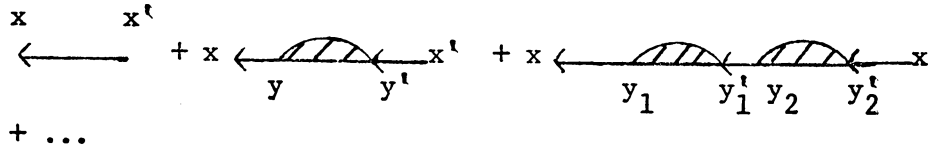
$$+ \int d^4y d^4y'\,iG_o(x,y)\left(\frac{-i}{\hbar}v(y'-y)\right)iG_o(y,y')iG_o(y',x')$$

$$+ \ldots + \int d^4y_1 d^4y_1' d^4y_2 d^4y_2'\,iG_o(x,y_1')\left(\frac{-i}{\hbar}v(y_1'-y_1)\right)iG_o(y_1',y_1)$$

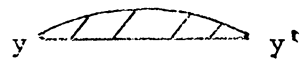
$$iG_o(y_1,y_2')\left(\frac{-i}{\hbar}v(y_2'-y_2)\right)iG_o(y_2',y_2)iG_o(y_2,x')$$

$$+ \ldots$$

Define a sub-diagram with either of the structures  or  (where  represents any allowed sub-diagram and all point labels in are integrated over) to be "proper" if it cannot be divided into two separate parts by breaking only one iG_o line. Then consider the sum of all proper diagrams, designated by a shaded half-circle (), and observe that by definition the series is regenerated by a sum of terms in which shaded half-circles are singly connected by iG_o lines. Specifically,



Letting

$-i\sum(y,y') =$ 

then

$$iG(x,x') = iG_o(x,x') + \int d^4y d^4y' iG_o(x,y)(-i)\sum(y,y')iG_o(y',x') + \ldots$$

or,

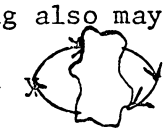
$$G(x,x') = G_o(x,x') + \int d^4y d^4y' G_o(x,y)\sum(y,y')G(y',x')$$

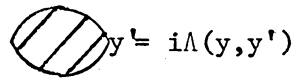
Note that $\sum(y,y')$ may be written

$$\sum(y,y') = \frac{1}{\hbar} B(y)\delta(y-y') + \sum{}'(y,y')$$

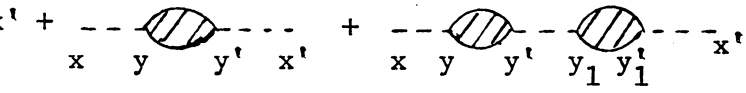
where $B(y)$ represents the sum of all proper sub-diagrams like 

$\sum'$ is then the remaining terms.

By using the technique shown above, the following also may be found. The sum of all sub-diagrams with the structure 

which are not separated into two parts by breaking one interaction line, denoted by 

$= i\Lambda(y,y')$, can be used to generate the series called the exact interaction, viz.,

$-\frac{i}{\hbar} V(x,x') =$ 

$+ \ldots$

or

$$V(x,x') = v(x-x') + \int d^4y d^4y' v(x-y)\Lambda(y,y')V(y',x') \qquad (11)$$

and similarly for the one-body potential:

$$W(x) = w(x) + \int d^4y d^4y' w(y)\Lambda(y,y')V(y',x) \qquad (12)$$

(note that $W(x)$ is only part of $B(x)$). For the present work, the

sum P = + + + ... is of primary interest.

This sum may be expressed in integral equation form as

$$P(x,x') = \Lambda(x,x') + \int d^4y d^4y' \Lambda(x,y) v(y-y') P(y',x') \quad . \tag{13}$$

Note that

$$V(x,x') = v(x-x') + \int d^4y d^4y' v(x-y) P(y,y') v(y'-x') \quad . \tag{14}$$

$P(x,x')$ is called the polarization propagator (PP) and $\Lambda(x,x')$ is called the proper polarization part (PPP).

2. The p-space Results

Next, we introduce explicitly the one particle basis functions into the Green function and perform a fourier transformation of the interaction:

$$G(x_1,\ldots x_n;x_1',\ldots,x_n') = (-i)^n \langle \Phi_o | T(\psi(x_1)\ldots\psi(x_n)\psi^+(x_n')\ldots\psi^+(x_1)S) | \Phi_o \rangle_{conn}$$

$$= \sum_{p_1 m_1} \cdots \sum_{p_n m_n} \sum_{p_1' m_1'} \cdots \sum_{p_n' m_n'} G(p_1 m_1,\ldots,p_n m_n;p_1' m_1',\ldots p_n' m_n') \phi_{p_1 m_1}(r_1)$$

$$e^{-i\frac{E_1 t_1}{\hbar}} \cdots \phi^*_{p_n' m_n'}(r_1') \, e^{i\frac{E_n' t_n'}{\hbar}}$$

where $p \equiv (p,E)$ and the sums over spin are not shown explicitly

$$G(p_1 m_1,\ldots p_n' m_n') \equiv \int d^4x_1 \ldots d^4x_n d^4x_1' \ldots d^4x_n' \phi^*_{p_1 m_1}(r_1) e^{i\frac{E_1 t_1}{\hbar}} \cdots$$

$$\phi_{p_n' m_n'}(r_n') e^{-i\frac{E_n' t_n'}{\hbar}} G(x_1,\ldots x_n') \tag{15}$$

and

$$v(y-y') = v(\vec{y}-\vec{y}')\delta(t-t') = \frac{1}{\Omega} \sum_q \int_{-\infty}^{\infty} \frac{d\nu}{2\pi\hbar} v(q) e^{i\vec{q}\cdot(\vec{y}-\vec{y}')} e^{-\frac{i\nu(t-t')}{\hbar}} \quad , \tag{16}$$

where

$$q \equiv (\vec{q},\nu) \qquad \text{and} \qquad y \equiv (\vec{y},t) \quad ,$$

and Ω is the periodic-box volume of the system. These transforms are now introduced into the perturbation series, each term is simplified as much as possible by carrying out internal space-time integrations, and it is found that the series for $G(p_1m_1,\ldots,p'_nm'_n)$ is represented by the same diagrams as before if we re-label each diagram and accordingly:

(a) for each element $\overset{n}{\leftarrow}\!\!\!-\!\!\!-\overset{p}{}\!\!\!-\!\!\!-\overset{n}{}$ write

$$iG_o(p,n);$$

(b) for each element $\leftarrow\!\!-\!\!-\overset{q}{}\!\!-\!\!-$ write

$$-\frac{i}{h}\,v(q);$$

(c) for each element $\leftarrow\!\!-\!\!-\overset{q}{}\!\!-\!\!-\!\!\bigcirc$ write

$$-\frac{i}{h}\,w(q);$$

(d) include (-1) factors as before;

(e) sum over all internal $\vec{p}$'s and $\vec{q}$'s and integrate over all internal E's and ν's;

(f) for each vertex $\overset{q}{\underset{pn \qquad p'n'}{}}$ write

the "vertex factor"

$$\int_{-\infty}^{\infty} d^3r\phi^*_{p'n'}(\vec{r})e^{i\vec{q}\cdot\vec{r}}\phi_{pn}(\vec{r})\int_{-\infty}^{\infty} dt\,e^{\frac{i(E'-E-\nu)t}{\hbar}} \quad .$$

In the Bloch case, the vertex factors (3 space part) become

$$\langle p',n'|e^{iq\cdot r}|p,n\rangle = \int_{-\infty}^{\infty} d^3r\phi^*_{p'n'}(r)e^{iq\cdot r}\phi_{pn}(r)$$

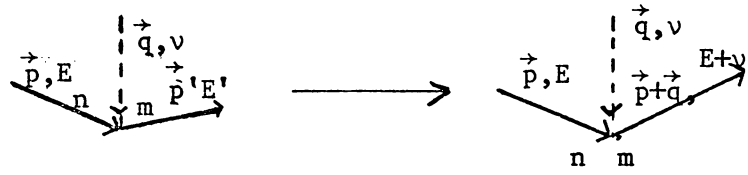
$$= \sum_{i=1}^{N} \int_{\text{ith cell}} d^3r \phi^*_{p'n'}(r) e^{iq\cdot r} \phi_{pn}(r)$$

$$= \frac{N}{\Omega} \sum_G \delta_{p'-p-q,G} \int_{\text{oth cell}} d^3r U^*_{p'n'}(r) e^{-iG\cdot r} U_{pn}(r) \qquad (17)$$

where G is a reciprocal lattice vector and N is the number of electrons in Ω. The time integral is

$$\int_{-\infty}^{\infty} dt\, e^{i\frac{(E'-E-\nu)t}{\hbar}} = 2\pi\hbar\delta(E'-E-\nu) \quad . \qquad (18)$$

(Note that $\phi_{pn}(r) = \frac{1}{\Omega^{1/2}} e^{ip\cdot r} U_{pn}(r)$ has been used explicitly). Thus a four-momentum conservation principle can be applied; i.e.,



(sum on G implied in the vertex factor) where $\delta_{p',p+q+G}\delta(E'-E-\nu)$ is used to eliminate $\sum_{p'}\int dE'$. $G_o(p,n)$, the fourier transform of the unperturbed one-particle Green's function is given by

$$G_o(p,n) = \frac{f_{pn}}{E - \varepsilon_{pn} - i\delta} + \frac{(1 - f_{pn})}{E - \varepsilon_{pn} + i\delta} \qquad (18a)$$

where ε_{pn} are the one-particle Bloch energies. The Fermi factor, f_{pn}, is

$$f_{pn} = 0 \quad \text{if} \quad \varepsilon_{pn} > \varepsilon_F, \text{ the Fermi energy}$$

$$= 1 \quad \text{if} \quad \varepsilon_{pn} < \varepsilon_F$$

Now introducing the fourier transform of the PP,

$$P(x,x') = \frac{1}{\Omega^2} \sum_q \sum_{q'} P(q,t;q',t') e^{iq\cdot r} e^{-iq'\cdot r'} \qquad (19)$$

along with the density operator

$$\rho(x) = \psi^{+}(x)\psi(x)$$

and

$$\rho(x) = \frac{1}{\Omega}\sum_{q} e^{iq\cdot r}\rho(q,t) \quad ,$$

it is a straightforward matter[1] to show that

$$P(x,x') = -i\langle\Psi_o|T(\rho(x')\rho(x))|\Psi_o\rangle = -i\langle\Phi_o|T(\rho(x')\rho(x)S)|\Phi_o\rangle_{conn} \tag{20}$$

and

$$P(q,t;q',t') = -i\sum_{G}\langle\Psi_o|T(\rho^{+}(q,t')\rho(q+G,t))|\Psi_o\rangle\delta_{q',q+G} \tag{21}$$

The time dependence of P is found by noting that

$$\langle\Psi_o|T(\rho^{+}(q',t')\rho(q,t))|\Psi_o\rangle = \langle\Psi_o|T(e^{iHt'}\rho^{+}(q',o)e^{-iHt'}e^{iHt}\rho(q,o)e^{-iHt})|\Psi_o\rangle$$

$$= \langle\Psi_o|T(\rho^{+}(q',T)\rho(q,o))|\Psi_o\rangle \tag{21a}$$

$$= \langle\Psi_o|T(\rho^{+}(q',\tfrac{T}{2})\rho(q,-\tfrac{T}{2}))|\Psi_o\rangle \tag{21b}$$

where $T \equiv t' - t$. Finally we introduce the following time fourier transformation:

$$P(q,q';t-t') = \int_{\infty}^{\infty}\frac{d\nu}{2\pi\hbar}P(q,q',\nu)e^{-i\frac{\nu(t-t')}{\hbar}} \tag{22}$$

Some analytic properties of $P(q,q',\nu)$ are presented in Appendix A.

III. THE PLASMON

1. Plasmon Energy and Linewidth

A system of particles interacting via the long-range coulomb interaction can exhibit a collective motion which is called plasma oscillation. Classically, a momentary charge density fluctuation in the system of amount $Ne\Delta x$ will be restored by a force arising from the resultant polarization field. Specifically, for a system of volume Ω with N particles of mass m, charge e, and polarization field $\frac{4\pi Ne\Delta x}{\Omega}$ associated with a density fluctuation,

$$m\ddot{\Delta x} = -e\left(\frac{4\pi Ne\Delta x}{\Omega}\right) = -m\omega_{p\ell}^2 \Delta x \quad .$$

Thus, a natural frequency $\omega_{p\ell}$ is found and is called the plasma frequency. Consider the fourier transform of the density operator $\rho(x) \equiv \psi^+(x)\psi(x)$:

$$\rho_q \equiv \int d^3x \rho(x) e^{-iq\cdot x}$$

and

$$\rho(x) = \frac{1}{\Omega} \sum_q \rho_q e^{iq\cdot x} \quad .$$

Since $\rho_o = \int d^3x \rho(x) = N$, then

$$\rho(x) = \frac{N}{\Omega} + \frac{1}{\Omega} \sum_{q \neq 0} \rho_q e^{iq\cdot x} \qquad (23)$$

which shows that the density fluctuation about the average is given by the second term. The fourier transform ρ_q for q not zero is called the density fluctuation operator. Note that

$$\rho_q = \sum_{k,m,n} (km|k+q,n) C^{+}_{km} C_{k+q,n} \quad , \tag{24}$$

where

$$(km|k+q,n) \equiv \frac{N}{\Omega} \int_{\text{unit cell}} d^3 r U^{*}_{km}(r) U_{k+qn}(r)$$

According to the perturbation theory presented earlier, the eigenstates of the complete Hamiltonian at t = 0 are to be generated via the interaction picture U matrix from the eigenstates of the non-interacting (unperturbed) system at $t = -\infty$. More specifically, if $\Phi_{\mu\nu}$ is the unperturbed eigenstate containing μ particles and ν holes, then $\psi_{\mu\nu}$ is an eigenstate of the full Hamiltonian containing μ particles and ν holes where

$$\psi_{\mu\nu} = U(0, -\infty)\Phi_{\mu\nu} \quad .$$

Since collective behavior cannot exist without particle interactions, some linear combination of unperturbed eigenstates must be adiabatically transformed to yield the plasmon excited state. The obvious choice is that linear combination generated when the density fluctuation operator is applied to the unperturbed ground state, i.e.,

$$\rho_q |\Phi_o\rangle \quad .$$

In Chapter I, the polarization propagator was introduced. Using (21b) and defining $P(q,t'-t) \equiv P(q,q;t'-t)$, $T = t'-t$, then

$$P(q,T) = \frac{-i}{\Omega} \langle \psi_o | T(\rho^{+}_q(\tfrac{T}{2}) \rho_q(-\tfrac{T}{2})) | \psi_o \rangle$$

(ρ_q's in the Heisenberg picture)

$$= \frac{-i}{\Omega} \langle \Phi_o | T(\rho_q^+(\tfrac{T}{2})\rho_q(-\tfrac{T}{2})S) | \Phi_o \rangle_{conn} \qquad (25)$$

(ρ_q's in the interaction picture). This may be written as

$$P(q,T) = -\frac{i}{\Omega} \frac{\langle \Phi_o | T(\rho^+(q,\frac{T}{2})\rho(q,-\frac{T}{2})S) | \Phi_o \rangle \text{ (all diagrams)}}{\langle \Phi_o | S | \Phi_o \rangle} \qquad (25a)$$

From DuBois[20] eq. 3.4a and 3.8 ($\hbar = 1$ in the following)

$$\langle \Phi_o | S | \Phi_o \rangle = e^{-iL}$$

where

$$E_o - \varepsilon_o = \lim_{T \to \infty} \frac{L}{T}$$

Here, E_o is the exact ground state energy and ε_o is the unperturbed ground state energy. Thus, if $T \to \infty$, then[21]

$$P(q,T) = \frac{-i}{\Omega} e^{i(E_o-\varepsilon_o)T} \langle \Phi_o | \rho_I^+(q,\tfrac{T}{2}) U(\tfrac{T}{2},-\tfrac{T}{2}) \rho_I(q,-\tfrac{T}{2}) | \Phi_o \rangle$$

$$= \frac{-i}{\Omega} e^{i(E_o-\varepsilon_o)T} \langle \Phi_o | e^{iH_o\frac{T}{2}} \rho_s^+(q) e^{-iH_o\frac{T}{2}} U(\tfrac{T}{2},-\tfrac{T}{2}) e^{iH_o\frac{(-T)}{2}} \rho_s(q) e^{-iH_o\frac{(-T)}{2}} | \Phi_o \rangle$$

$$= \frac{-i}{\Omega} e^{iE_oT} \langle \Phi_o | \rho_s^+(q) e^{-iH_o\frac{T}{2}} U(\tfrac{T}{2},-\tfrac{T}{2}) e^{iH_o\frac{(-T)}{2}} \rho_s(q) | \Phi_o \rangle$$

Observe that $P(q,T)$ is proportional to the scalar product of the Schrodinger state

$$\rho_q^s | \Phi_o \rangle$$

at time $\frac{-T}{2}$ with its adiabatic transform at time $\frac{T}{2}$. The adiabatic transformation is accomplished by converting to the interaction picture, performing the transformation, then converting back to the Schrodinger picture.

In general for any Schrodinger state χ^s,

$$\chi^s(t_2) = e^{-iH(t_2 - t_1)}\, \chi^s(t_1)$$

and, in particular, if χ^s is an approximate eigenstate of H with energy E and linewidth Γ such that $\frac{\Gamma}{E} << 1$ and $\Gamma\Delta t << 1$ where $\Delta t = t_2 - t_1$ then

$$\langle\chi^s(t_1)|\chi^s(t_2)\rangle = e^{-i(E - i\,\Gamma/2)\Delta t}\, \langle\chi^s(t_1)|\chi^s(t_1)\rangle \quad .$$

So, it is seen that if the adiabatic transform of the density fluctuation state is an approximate eigenstate of the full Hamiltonian, then P(q,T) will have time dependence

$$e^{-i(E - E_o - i\,\Gamma/2)T} \tag{26}$$

Now, since

$$P(q,t-t') = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi}\, P(q,\nu) e^{-i\nu(t-t')} \tag{27}$$

and, from the analytic properties (Appendix A),

$$P(q,\nu) = \frac{1}{\pi}\int_o^{\infty} d\nu' \, \frac{2\nu'}{(\nu' - i\eta)^2 - \nu^2}\, \mathrm{Im}P(q,\nu') \tag{28}$$

$$= -\frac{1}{\pi}\int_o^{\infty} d\nu' \mathrm{Im}P(q,\nu')\left[\frac{1}{\nu - (\nu' - i\eta)} - \frac{1}{\nu + (\nu' - i\eta)}\right] \quad ,$$

then

$$P(q,t-t') = -\frac{1}{\pi}\int_o^{\infty} d\nu' \mathrm{Im}P(q,\nu') \int_{-\infty}^{\infty} \frac{d\nu}{2\pi}\, e^{-i\,(t-t')}\left[\frac{1}{\nu-(\nu'-i\eta)} - \frac{1}{\nu-(-\nu'+i\eta)}\right] ,$$

or, closing the contour in the lower half ν-plane,

$$P(q,t-t') = \frac{i}{\pi}\int_o^{\infty} d\nu' \mathrm{Im}P(q,\nu') e^{-i\nu'(t-t')} \quad .$$

We recall that, in the pair approximation[22], neglecting local field effects,

$$P(q,\nu) = \frac{\Lambda(q,\nu)}{1-v(q)\Lambda(q,\nu)} = \frac{\Lambda^r+i\Lambda^i}{1-v\Lambda^r-iv\Lambda^i} ,$$

where $Re\Lambda = \Lambda^r$ and $Im\Lambda = \Lambda^i$, so that

$$ImP(q,\nu) = \frac{\Lambda^i(q,\nu)}{(1-v(q)\Lambda^r(q,\nu))^2+(v(q)\Lambda^i(q,\nu))^2} ,$$

or

$$P(q,t-t') = \frac{i}{\pi}\int_0^\infty d\nu e^{-i\nu(t-t')}\frac{\Lambda^i(q,\nu)}{(1-v(q)\Lambda^r(q,\nu))^2+(v(q)\Lambda^i(q,\nu))^2} \quad (29)$$

The integrand in eq. (29) is sharply peaked at $\nu = \nu_o$ where

$$1-v(q)\Lambda^r(q,\nu_o) = 0 \quad (30)$$

provided $v(q)\Lambda^i(q,\nu_o)$ and $\nu_o(t-t')$ are appropriately small. Define $B(q,\nu-\nu_o)$ by

$$v(q)(\nu-\nu_o)B(q,\nu-\nu_o) \equiv 1-v(q)\Lambda^r(q,\nu)$$

so that

$$B(q,0) = -\frac{d}{d\nu}\Lambda^r(q,\nu)\Big|_{\nu=\nu_o} , \quad (31)$$

and define $\Gamma(q,\nu_o)$ by

$$\frac{\Gamma}{2} \equiv \frac{\Lambda^i(q,\nu_o)}{B(q,0)} . \quad (32)$$

The major contribution to the integral in eq. (29) occurs at $\nu = \nu_o$, thus this equation becomes

$$P(q,t-t') \simeq \frac{i}{\pi}\int_0^\infty d\nu e^{-i\nu(t-t')} \frac{B(q,o)\Gamma/2}{[v(q)(\nu-\nu_o)B(q,\nu-\nu_o)]^2+[v(q)B(q,o)\frac{\Gamma}{2}]^2}$$

$$= \frac{i}{\pi}\frac{e^{-i\nu_o(t-t')}}{(v(q))^2B(q,o)}\int_{\frac{-\nu_o}{\Gamma/2}}^\infty dx \frac{e^{-i\frac{\Gamma}{2}x(t-t')}}{x^2+1} \quad (33)$$

If $\frac{\Gamma}{2} << \nu_o$ (i.e., $|\Lambda^i(q,\nu_o)| << \nu_o|\frac{d}{d\nu}\Lambda^r(q,\nu_o)|$), then, using $\frac{\nu_o}{\Gamma/2} \to \infty$, the value of the integral in eq. (33) is

$$\pi e^{-\frac{\Gamma}{2}(t-t')}$$

so that

$$P(q,t-t') = \frac{i}{(v(q))^2B(q,o)} e^{-i\nu_o(t-t')}e^{-\frac{\Gamma}{2}(t-t')} \quad (34)$$

from eqs. (34) and (26), we infer that, in the limit as $t-t' \to \infty$,

$$E = E_o + \nu_o$$

That is, ν_o is the energy of the plasmon state with respect to the exact ground state and Γ is the linewidth of the plasmon state.

2. The Insulator Case

Now, in the pair approximation (without local field effects)[22],

$$i\Lambda(q) = \sum_{mn}\int\frac{d^3kdE}{(2\pi)^4} iG_o(k,m)iG_o(k+q,n)|(k+q,n|k,m)|^2(-1)$$

is the proper polarization part with G_o given by eq. (16a) in Chapter I; perform the indicated integration over E by applying Cauchy's theorem:

$$\Lambda(q) = \sum_{mn} \int \frac{d^3k}{(2\pi)^3} \cdot \frac{1}{2\pi i} \int_{\infty}^{\infty} dE \left[\frac{f_{km} f_{k+qn}}{(E-\varepsilon_{km}-i\delta)(E+\hbar\nu-\varepsilon_{k+qn}-i\delta)} + \right.$$

$$\frac{(1-f_{km})(1-f_{k+qn})}{(E-\varepsilon_{km}+i\delta)(E+\hbar\nu-\varepsilon_{k+qn}+i\delta)} +$$

$$\frac{f_{km}(1-f_{k+qn})}{(E-\varepsilon_{km}-i\delta)(E+\hbar\nu-\varepsilon_{k+qn}+i\delta)} +$$

$$\left. \frac{f_{k+qn}(1-f_{km})}{(E+\hbar\nu-\varepsilon_{k+q}-i\delta)(E-\varepsilon_{km}+i\delta)} \right] \quad | \, (k+qn|km) \, |^2 \, .$$

The first two terms give zero since the contour can be closed in the lower and upper half E plane respectively. Closing the contour in the upper half E plane in the last two integrals, the proper polarization part becomes

$$\Lambda(q) = \sum_{mn} \int \frac{d^3k}{(2\pi)^3} \left[\frac{f_{km}(1-f_{k+qn})}{\varepsilon_{km}-\varepsilon_{k+qn}+\hbar\nu+i\delta} + \frac{f_{k+q}(1-f_{km})}{\varepsilon_{k+q}-\varepsilon_{km}-\hbar\nu+i\delta} \right] | \, (k+qn|km) \, |^2$$

$$= \sum_{m} \lambda_{mm}(q,q) + \sum_{\substack{m \\ m \neq n}} \sum_{n} \lambda_{mn}(q,q) \qquad (35)$$

where $\lambda_{mn}(q)$ has an obvious definition.

Specializing to the perfect insulator or semiconductor case, $\lambda_{mm}(q,q)$ is zero since for each m, $\varepsilon_{k,m} \lesseqgtr \varepsilon_F$ for all k and therefore $f_{k,m}(1 - f_{k',m}) = 0$ for all k and k'. Furthermore, denoting all bands below ε_F by v_i (valence and core) and all bands above ε_F by c_j (conduction), the product $(m \neq n) f_{km}(1 - f_{kn}) = 0$ for all k, k' unless $m \varepsilon v_i$, $n \varepsilon c_j$ or vice-versa, i.e.,

$$\Lambda(q) = \sum_i \sum_j [\lambda_{v_i c_j}(q) + \lambda_{c_j v_i}(q)]$$

where

$$\lambda_{v_i c_j}(q) = \int \frac{d^3k}{(2\pi)^3} \left[- \frac{1}{\varepsilon_{k+qc_j} - \varepsilon_{kv_i} - \hbar\nu - i\delta} \right] |(k+qc_j|kv_i)|^2$$

$$\lambda_{c_j v_i}(q) = \int \frac{d^3k}{(2\pi)^3} \left[\frac{1}{\varepsilon_{k+qv_i} - \varepsilon_{kc_j} - \hbar\nu + i\delta} \right] |(k+qv_i|kc_j)|^2 \quad .$$

Setting $k' = k + q$, then, e.g.,

$$\lambda_{v_i c_j}(q) = \int_{Bz'} \frac{d^3k'}{(2\pi)^3} \frac{-1}{\varepsilon_{k'c_j} - \varepsilon_{k'-qv_i} - \hbar\nu - i\delta} |(k'c_j|k'-qv_i)|^2 \quad .$$

Note that the value of the integral is independent of the location in k space of the origin with respect to the integration volume.

Therefore,

$$\Lambda(q) = - \sum_{ij} \int_{Bz} \frac{d^3k}{(2\pi)^3} \left[\frac{|(kc_j|k-qv_i)|^2}{\varepsilon_{kc_j} - \varepsilon_{k-qv_i} - \hbar\nu - i\delta} + \frac{|(k+qv_i|kc_j)|^2}{\varepsilon_{kc_j} - \varepsilon_{k+qv_i} + \hbar\nu - i\delta} \right] . \quad (36)$$

Using $\frac{1}{x \pm i\delta} = PV \frac{1}{x} \mp \pi i \delta(x)$, the real and imaginary parts of Λ may be found (where PV denotes principal value):

$$\Lambda^r(q) = -\sum_{ij} PV \int_{Bz} \frac{d^3k}{(2\pi)^3} \left[\frac{|(kc_j|k-qv_i)|^2}{\varepsilon_{kc_j} - \varepsilon_{k-qv_i} - \hbar\nu} + \frac{|(k+qv_i|kc_j)|^2}{\varepsilon_{kc_j} - \varepsilon_{k+qv_i} + \hbar\nu} \right] \quad (37)$$

$$\Lambda^i(q) = -\pi \sum_{ij} \int \frac{d^3k}{(2\pi)^3} [\delta(\varepsilon_{kc_j} - \varepsilon_{k-qv_i} - \hbar\nu) |(kc_j|k-qv_i)|^2 +$$

$$\delta(\varepsilon_{kc_j} - \varepsilon_{k+qv_i} + \hbar\nu) |(k+qv_i|kc_j)|^2] \quad . \quad (38)$$

Note that the second term in Λ^i is zero for all $\nu \geq 0$. Furthermore, the principal value restriction may be relaxed in the second term of Λ^r (since the denominator never vanishes). If we can find solutions to the single particle Bloch equation, $\Lambda(q)$ can be calculated. Since exact solutions are not available, a simple model will be used in Chapter III for this calculation.

3. The Simplest Approximation

Before an explicit calculation of Λ is performed, some general features of the plasmon energy are worth noting. The essential observation is that typical interband transition energies for insulators are from 1 eV to 10 eV. Plasmon energies are generally 12 eV to 25 eV. Thus, one might expect that an approximation in which E(interband) << E(plasma) would prove useful. This, along with a number of other approximations will now be made in order to examine the plasmon dispersion relation. Using a result of first order (non-degenerate) "k·p" perturbation theory[23], viz.,

$$U_{k+qn} = U_{kn} + \frac{h}{m} \sum_i{}' \frac{U_{ki}(ki|q\cdot p|kn)}{\epsilon_{kn} - \epsilon_{ki}} \quad ,$$

we find

$$\frac{N}{\Omega} \int_{uc} d^3y U^*_{km}(y) U_{k-qn}(y) = -\frac{h}{m} \frac{(kn|q\cdot p|km)}{\epsilon_{kn} - \epsilon_{km}}$$

$$\frac{N}{\Omega} \int_{uc} d^3y U^*_{k+qn}(y) U_{km}(y) = \frac{h}{m} \frac{(kn|q\cdot p|km)}{\epsilon_{kn} - \epsilon_{km}} \quad .$$

Thus, to lowest order in q,

$$|(km|k-qn)|^2 = \frac{\hbar^2}{m^2\omega_{nm}^2}\,|(kn|q\cdot p|km)|^2 = |(k+qn|km)|^2 \quad , \tag{39}$$

where $\omega_{nm} = \varepsilon_{kn} - \varepsilon_{km}$, so that, to order q^2,

$$\Lambda^r = -\sum_{ij} PV \int_{Bz} \frac{d^3k}{(2\pi)^3}\frac{\hbar^2}{m^2}\,\frac{|(kc_j|q\cdot p|kv_i)|^2}{\omega_{ji}^2}\left[\frac{1}{\varepsilon_{kc_j}-\varepsilon_{kv_i}-\hbar\nu} + \frac{1}{\varepsilon_{kc_j}-\varepsilon_{kv_i}+\hbar\nu}\right]$$

$$= -\sum_{ij} PV \int_{Bz} \frac{d^3k}{(2\pi)^3}\frac{\hbar^2}{m^2}\,\frac{|(kc_j|q\cdot p|kv_i)|^2}{\omega_{ji}}\,\frac{2}{\omega_{ji}^2-\hbar^2\nu^2} \tag{40}$$

and

$$\Lambda^i = -\frac{\pi\hbar^2}{m^2}\sum_{ij}\int_{Bz}\frac{d^3k}{(2\pi)^3}\,\frac{|(kc_j|q\cdot p|kv_i)|^2}{\omega_{ji}^2}\,\delta(\omega_{ji}-\hbar\nu) \quad . \tag{41}$$

Now, rearrange $\sum_{ij}$ into those terms for which ν is either less or greater than ω_{ji} and those where, at some point in the Bz, $\nu=\omega_{ji}$. Thus, the sum over i,j is broken up into three terms:

$$\Lambda^r = \underset{(\hbar\nu<\omega_{ji})}{\sum_{ij}\lambda_{ij}^r} + \underset{(\hbar\nu=\omega_{ji}\text{ for some k})}{\sum_{ij}\lambda_{ij}^r} + \underset{(\hbar\nu>\omega_{ji})}{\sum_{ij}\lambda_{ij}^r} \tag{40a}$$

$$\Lambda^i = \underset{(\hbar\nu=\omega_{ji}\text{ for some k})}{\sum_{ij}\lambda_{ij}^i}$$

The usual assumption is now made, (see Pines[13] and Brout and Carruthers[24]), namely, that the band structure is such that the plasma frequency ν_o has a value different from any interband transition frequency of importance. That is, the second term of eq. (40a) for Λ^r maybe neglected because the matrix elements are suitably small. The further assumption is made that

$$\omega_{\text{conduction,valence}} << h\nu_o << \omega_{\text{conduction,core}}$$

and the denominators of the remaining terms in eq. (40) are than appropriately expanded:

for the first term in eq. (40a):

$$\frac{1}{\omega_{ji}^3\left(1 - \frac{\hbar^2\nu^2}{\omega_{ji}^2}\right)} \simeq \frac{1}{\omega_{ji}^3}\left(1 + \frac{\hbar^2\nu^2}{\omega_{ji}^2}\right)$$

for the third term in eq. (40a):

$$\frac{1}{-\omega_{ji}\hbar^2\nu^2\left(1 - \frac{\omega_{ji}^2}{\hbar^2\nu^2}\right)} \simeq \frac{1}{-\omega_{ji}^2\hbar^2\nu^2}\left(1 + \frac{\omega_{ji}^2}{\hbar^2\nu^2}\right) .$$

Now, defining

$$f_{ij}(k) \equiv \frac{2\hbar^2}{mq^2}\,\frac{|(kj|q\cdot p|ki)|^2}{\omega_{ji}} \tag{42}$$

(note that f_{ij} is independent of q), the real part of the PP is

$$\Lambda^r = \frac{-q^2}{m}\sum_{\text{core}}\sum_{\text{conduction}}\int_{Bz}\frac{d^3k}{(2\pi)^3}\,\frac{f_{\text{core,cond.}}}{\omega^2_{\text{cond,core}}}\left(1 + 0\left(\frac{\hbar^2\nu^2}{\omega^2_{\text{cond,core}}}\right)\right)$$

$$+ \frac{q^2}{m} \sum_{\text{valence}} \sum_{\text{conduction}} \int_{Bz} \frac{d^3k}{(2\pi)^3} f_{\text{val.,cond.}}$$

$$(1 + \frac{\omega^2_{\text{val.,cond.}}}{\hbar^2 \nu^2})$$

and the plasmon dispersion relation becomes

$$1 - v(q)\Lambda^r(q,\nu_o) = 0 \tag{43}$$

$$= 1 + 4\pi\alpha_{\text{core}} - \frac{4\pi e^2}{m\nu_o^2} \sum_{\text{val}} \sum_{\text{cond}} \int_{Bz} \frac{d^3k}{(2\pi)^3} f_{\text{val.,cond.}}$$

$$- \frac{4\pi e^2}{m\nu_o^4} \sum_{\text{val}} \sum_{\text{cond}} \int_{Bz} \frac{d^3k}{(2\pi)^3} f_{\text{val,cond.}} \omega^2_{\text{val,cond.}} \quad ,$$

where we have defined

$$4\pi\alpha_{\text{core}} = \frac{4\pi e^2}{m} \sum_{\text{core}} \sum_{\text{conduction}} \int \frac{d^3k}{(2\pi)^3} \frac{f_{\text{core,cond.}}}{\omega^2_{\text{core,cond.}}} \tag{44}$$

It can be shown (Pines[13]) that the quantities $f_{\text{val.,cond.}}$ obey the following sum rule, where N_{VAL} is the number of electrons in the valence bands:

$$\sum_{\text{val}} \sum_{\text{cond.,k}} f_{\text{val,}}(k)_{\text{cond}} = N_{VAL} + \sum_{\text{val}} \sum_{\text{core,k}} f_{\text{core,}}(k)_{\text{val.}} \tag{45}$$

Define an $\tilde{N}_{VAL}$ by

$$\tilde{N}_{VAL} = N_{VAL} + \sum_{\text{val}} \sum_{\text{core,k}} f_{\text{core,val}} \quad ; \tag{46}$$

then calling $1 + 4\pi\alpha_{core} = K_{core}$ we find, using $\int \frac{d^3k}{(2\pi)^3} = \frac{1}{\Omega} \sum_k$,

$$0 = K_{core} - \frac{4\pi e^2 \tilde{N}_{VAL}}{m\Omega\nu_o^2} - \frac{4\pi e^2}{m\nu_o^4} \sum_{val} \sum_{cond} \int \frac{d^3k}{(2\pi)^3}$$

$$f_{val.,cond} \omega^2_{val.,cond.}$$

Thus, if the second term is neglected,

$$\nu_o^2 = \frac{4\pi e^2 \tilde{N}_{VAL}}{m\Omega K_{core}} , \tag{47}$$

i.e., ν_o is the ordinary plasma frequency for $\tilde{N}_{VAL}$ electrons in a medium of dielectric constant K_{core}. Keeping the second term and using $\tilde{\nu}^2_{val} \equiv \frac{4\pi \tilde{N}_{VAL} e^2}{m\Omega}$, we find

$$\nu_o^2 \simeq \frac{\tilde{\nu}^2_{val}}{K_{core}} \left(1 + \frac{4\pi e^2 K_{core}}{\tilde{m}\tilde{\nu}^4_{val}} \sum_{val} \sum_{cond} \int \frac{d^3k}{(2\pi)^3}\right.$$

$$\left. f_{val.,cond.} \omega^2_{val.,cond}\right) \tag{48}$$

Since we have assumed that the Bloch factor is negligible for those bands for which $\hbar\nu_o \simeq \omega_{ji}$, Λ^i is negligible in this approximation. Results similar to those of Horie[24] and Miyakawa[25] can be obtained if we approximate

$$\frac{4\pi e^2 K_{core}}{\tilde{m}\tilde{\nu}^4_{val}} \sum_{val} \sum_{cond} \int \frac{d^3k}{(2\pi)^3} f_{val.,cond.} \omega^2_{val.,cond.}$$

$$- \frac{\overline{\omega^2_{val.,cond.}}}{\tilde{\nu}^2_{val}} K_{core}$$

and

$$\tilde{N}_{Val} \sim N_{VAL}$$

where $\overline{\omega^2_{val}}$ is an average value for the interband transition energy. The result is

$$\nu_o^2 = \frac{\nu^2_{val}}{K_c} + \overline{\omega^2_{val.,cond.}} \qquad (49)$$

Note that this expression does not account for the enhancement of N_{VAL} by the core bands. K_c may be calculated using experimental values for the electronic polarizability[26]. Results of calculations for ν_o using eq. (49) are presented in Table I (Chapter IV) for several solids. Generally, the agreement with experiment is fair. We will find, however, that the model presented in Chapter IV yields, on the whole, better agreement with experiment.

IV. PLASMON ENERGIES OF A MODEL INSULATOR

1. The Isotropic Band Model

The work of Horie[24], Pines[13], Brout and Carruthers[24] and Miyakawa[25] have already been mentioned. We arrived at the result eq. (49) by a combination of approximations used by these authors. In addition, Wilson[27] studies the shift of the plasmon energy from the free plasmon value by considering a two band model and phenomenological equations for the frequency dependent dielectric function. He finds the plasmon energy is increased when the free

plasmon energy lies above the interband transition energy region and is decreased when it lies below; if the free plasmon energy lies within the interband transition energy region, it turns out that the location of the plasmon root depends on the details of the integrand in eq. (37).

We now wish to carry out somewhat more involved numerical calculations of plasmon energies (and lifetimes) using a band model which in particular avoids the assumptions made above concerning the magnitude of the plasmon energy relative to the important interband transition energies. A simple isotropic band model such as the one used by Fry[16] may be employed for this purpose. Using a tight-binding approximation for the wave functions of the valence bands and an OPW for the (single) conduction band, $\Lambda(q)$ may be evaluated in the long wavelength (small q) limit.

The Bz is approximated by a sphere of radius k_B, i.e.

$$\frac{4}{3}\pi k_B^3 = \Omega_{Bz} = \frac{(2\pi)^3}{\frac{V}{N}} \tag{50}$$

Furthermore, the valence band wave functions are taken as

$$\psi_i(k,r) \equiv \frac{1}{\sqrt{N}} \sum_\nu e^{ik\cdot R_\nu} U_i(r - R_\nu), \quad i = 1,2,3 \tag{51}$$

and the (unnormalized) conduction band wave function is

$$\psi_c(k,r) \equiv \frac{e^{ik\cdot r}}{\sqrt{\Omega}} - \sum_i \mu_i(k)\psi_i(k,r) \quad , \tag{52}$$

where the μ_i are the orthogonalization coefficients given by

$$\mu_i(k) = \frac{1}{\sqrt{\Omega}} \int_{\text{all space}} e^{ik\cdot r} \psi_i^*(k,r) d^3r \tag{53}$$

and $U_i(r) = U(r)\theta_i(\theta,\phi)$, where θ_i is the Y_1^i spherical harmonic, and

$$U(r) = \left[\frac{(2\delta)^5}{24}\right]^{1/2} re^{-\delta r} \tag{54}$$

where δ is a parameter to be determined. Now to normalize $\psi_c(k,r)$ proceed according to Fry (op.cit.): using eq. (52), the normalization constant is found to be

$$\int d^3r \psi_c^*k(r)\psi_c k(r) = A$$
$$= 1 - \sum_{i=1}^{3} |\mu_i|^2 \quad . \tag{55}$$

When (51) is employed in (53), we find

$$\mu_i(k) = \frac{1}{(\Omega N)^{1/2}} \sum_\nu \int_\Omega d^3r U^*_i(r-R_\nu) e^{ik\cdot(r-R_\nu)}$$
$$= \left(\frac{N}{\Omega}\right)^{1/2} \int_\Omega d^3r U^*_i(r) e^{ik\cdot r} \quad .$$

Now,

$$e^{ik\cdot r} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{\ell m} j_\ell(kr) Y_\ell^m(\theta_k,\phi_k)$$

so that

$$\mu_i(k) = 4\pi \left(\frac{N}{\Omega}\right)^{1/2} i\, Y_1^i(\theta_k,\phi_k) \int_o^\infty j_1(kr) U^*(r) r^2 dr$$

or[16]

$$\mu_o = 4\pi \left(\frac{N}{\Omega}\right)^{1/2} \frac{3}{4\pi} \cos\theta \left[\frac{(2\delta)^5}{24}\right]^{1/2} \frac{8\delta k}{(\delta^2+k^2)^3} \tag{56a}$$

$$\mu_{-1} = 4\pi \left(\frac{N}{\Omega}\right)^{1/2} \frac{3}{8\pi} \sin\theta e^{-i\phi} \left[\frac{(2\delta)^5}{24}\right]^{1/2} \frac{8\delta k}{(\delta^2+k^2)^3} \tag{56b}$$

$$\mu_1 = -4\pi\left(\frac{N}{\Omega}\right)^{1/2} \frac{3}{8\pi} \sin\theta e^{i\phi}\left[\frac{(2\delta)^5}{24}\right]^{1/2} \frac{8\delta k}{(\delta^2+k^2)^3} \quad . \tag{56c}$$

Thus, when (56a,b,c) are used in (55), we find

$$A = 1 - 8\pi \frac{N}{\Omega} \frac{(2\delta)^7 k^2}{(\delta^2 + k^2)^6} \tag{57}$$

And, in this model eqs. (37) and (38) for the real and imaginary parts of the PPP in pair approximation without local-field effects are

$$\Lambda^r(q) = -2 \sum_{i=1}^{3} PV \int_{Bz} \frac{d^3k}{(2\pi)^3} \frac{|(kc|k-qv_i)|^2}{\varepsilon_{kc}-\varepsilon_{k-qv_i}-\hbar\nu}$$

$$-2 \sum_{i=1}^{3} PV \int_{Bz} \frac{d^3k}{(2\pi)^3} \frac{|(k+qv_i|kc)|^2}{\varepsilon_{kc}-\varepsilon_{k+qv_i}+\hbar\nu} \tag{58}$$

$$\Lambda^i(q) = -2\pi \sum_{i=1}^{3} \int_{Bz} \frac{d^3k}{(2\pi)^3} \delta(\varepsilon_{kc}-\varepsilon_{k-qv_i}-\hbar\nu)|(kc|k-qv_i)|^2 \quad , \tag{59}$$

where factors of 2 appear from sums over spins which have heretofore been implied but suppressed.

Since the primary case of interest is $q \to 0$ (i.e. $qa_o << 1$, where a_o is a lattice parameter), this limit is taken in what follows. Now, introduce the following approximations for the energy denominators:

$$\varepsilon_{kc}-\varepsilon_{k\pm qv_i} \pm \hbar\nu \simeq E_c k^2 - \beta_i + E_i' k^2 \pm \hbar\nu$$

$$= |\beta_i|(\Delta_i x^2 + 1 \pm W_i) \equiv E_i \tag{60}$$

where we have defined

$$\Delta_i \equiv \frac{E_c + E_i'}{|\beta_i|} k_B^2 \quad , \qquad i = 1,2,3$$

$$W_i = \frac{h\nu}{|\beta_i|}$$

$$x = \frac{k}{k_B}$$

Furthermore, to lowest order in q (i.e. q^2), with $\vec{q}$ taken to lie along the z-direction in $\vec{k}$ space (see diagram below) and noting that

$$(k+qv_z|kc) = \frac{N}{\Omega} \int_{\text{unit cell}} d^3r U^*_{k+qv_z}(r) U_{kc}$$

$$= \int_{\Omega} d^3u \psi^*_{k+q\cdot v_z}(y) e^{iq\cdot y} \psi_{kc}(y)$$

$$= \langle \psi_{k+qv_z} | e^{iq\cdot y} | \psi_{kc} \rangle \quad ,$$

the Bloch factors appearing in (58) and (59) may be calculated.

Using eqs. (51), (52), (54), (56a,b,c), (57), and some algebra we find

$$|(k+qv_z|kc)|^2 = |(kc|k-qv_z)|^2$$

$$= 8\pi\frac{N}{\Omega}(2\delta)^7 \frac{q^2}{(\delta^2+k^2)^6} \frac{1}{[1-8\pi\frac{N}{\Omega}\frac{(2\delta)^7 k^2}{(\delta^2+k^2)^6}]} [1 - \frac{6k^2\cos^2\theta^2}{\delta^2+k^2}] \qquad (61)$$

and

$$|(k+qv_x|kc)|^2 = |(k+qv_y|kc)|^2 = |(kc|k-qv_x)|^2 = |(kc|k-qv_y)|^2$$

$$= 4\pi\frac{N}{\Omega}(2\delta)^7 \frac{q^2}{(\delta^2+k^2)^8} \frac{1}{[1-8\pi\frac{N}{\Omega}\frac{(2\delta)^7 k^2}{(\delta^2+k^2)^6}]} 36k^4\cos^2\theta\sin^2\theta \ . \qquad (62)$$

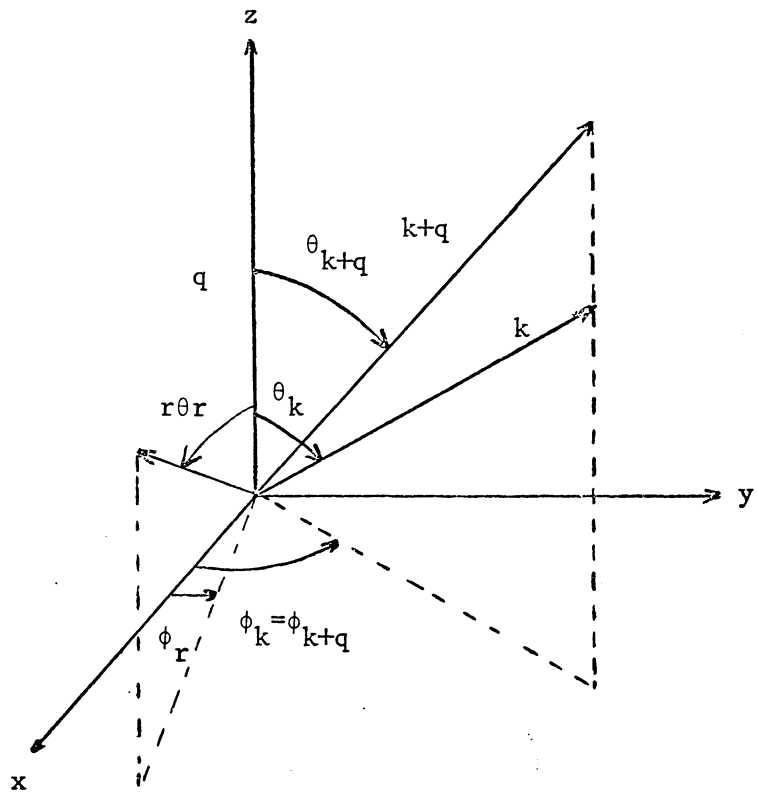


Figure 1. Angular Relationships

These results are now used for the matrix elements and the energy denominators in the present expression for $\Lambda(q)$ i.e., (58) and (59).

Let

$$C \equiv 8\pi\frac{N}{V}\frac{1}{k_B^3}\left(2\frac{\delta}{k_B}\right)^7 = \frac{4}{3\pi}(2\Delta)^7$$

where

$$\Delta \equiv \frac{\delta}{k_B}$$

Then, upon employing the spherical Bz approximation, we obtain

$$\lim_{q\to o}\Lambda^r(q) = -PV\int_o^1\frac{x^2dx}{(2\pi)^2}k_B^3\sum_{i=1}^{2}\frac{1}{E_i}\int_{-1}^{1}d\mu\, 36\frac{C}{2}\cdot 2\cdot\frac{q^2}{k_B^2}$$

$$x^4\mu^2(1-\mu^2)\frac{1}{1-\frac{Cx^2}{(\Delta^2+x^2)^6}}\cdot\frac{1}{(\Delta^2+x^2)^8}$$

$$-PV\int_o^1\frac{x^2dx}{(2\pi)^2}k_B^3\frac{1}{E_3}\int_{-1}^{1}d\mu C\cdot 2\frac{q^2}{k_B^2}$$

$$\left[1-\frac{6x^2\mu^2}{\Delta^2+x^2}\right]^2\frac{1}{1-\frac{Cx^2}{(\Delta^2+x^2)^6}}\cdot\frac{1}{(\Delta^2+x^2)^6} \qquad (63)$$

$$\lim_{q\to o}\Lambda^i(q) = -\pi\int_o^1\frac{x^2dx}{(2\pi)^2}k_B^3\sum_{i=1}^{2}\delta(E_i)\int_{-1}^{1}d\mu \quad \text{(as in first term above)}$$

$$-\pi\int_o^1\frac{x^2dx}{(2\pi)^2}k_B^3\delta(E_3)\int_{-1}^{1}d\mu \quad \text{(as in second term above)} \qquad (64)$$

The integrals over μ can be done immediately, and calling

$$\lim_{q\to o} \Lambda^{r,i}(q) = \Lambda^{r,i}(\nu) \quad ,$$

eq. (63) and (64) for $\Lambda^r(\nu)$ and $\Lambda^i(\nu)$ become

$$\Lambda^r(\nu) = -q^2 \frac{Ck_B}{(2\pi)^2} \left[36\cdot\frac{4}{15}\left(\frac{1}{\beta_1} I_1(3,8)+ \frac{1}{\beta_2} I_2(3,8)\right)\right.$$

$$\left. + \frac{4}{\beta_3}\left(I_3(1,6) - \frac{12}{3} I_3(2,7) + \frac{36}{5} I_3(3,8)\right)\right] \tag{65}$$

$$\Lambda^i(\nu) = -q^2 \frac{\pi Ck_B}{(2\pi)^2} \left[36\cdot\frac{4}{15}\left(\frac{1}{\beta_1} D_1(3,8) + \frac{1}{\beta_2} D_2(3,8)\right)\right.$$

$$\left. + \frac{4}{\beta_3}\left(D_3(1,6) - \frac{12}{3} D_3(2,7) + \frac{36}{5} D_3(3,8)\right)\right] \tag{66}$$

where

$$I_i(s,\sigma) \equiv P_i(s,\sigma) + R_i(s,\sigma) \tag{67}$$

$$P_i(s,\sigma) \equiv PV \int_o^1 dx x^{2s} \frac{1}{(\Delta i x^2+1-W_i)} \cdot \frac{1}{1-\frac{Cx^2}{(\Delta^2+x^2)^6}} \cdot \frac{1}{(\Delta^2+x^2)^\sigma} \tag{67a}$$

$$R_{\beta i}(s,\sigma) \equiv \int_o^1 dx x^{2s} \frac{1}{(\Delta_i x^2+1+W_i)} \cdot \frac{1}{1-\frac{Cx^2}{(\Delta^2+x^2)^6}} \cdot \frac{1}{(\Delta^2+x^2)^\sigma} \tag{67b}$$

$$D_{\beta i}(s,\sigma) \equiv \int_o^1 dx x^{2s} \delta[\beta i(\Delta_i x^2+1-W_i)] \cdot \frac{1}{1-\frac{Cx^2}{(\Delta^2+x^2)^6}} \cdot \frac{1}{(\Delta^2+x^2)^\sigma} \tag{67c}$$

Now, define

$$g(x^2) = x^{2s} \quad \frac{1}{1 - \frac{Cx^2}{(\Delta^2+x^2)^6}} \quad \cdot \quad \frac{1}{(\Delta^2+x^2)^\sigma}$$

then

$$\int_0^1 dx \frac{g(x^2)}{(\Delta_i x^2+1-W_i)} = \frac{1}{2\Delta_i} \int_0^1 dy \frac{g(y)}{y^{1/2}} \cdot \frac{1}{y - \frac{W_i - 1}{\Delta_i}}$$

$$= \frac{1}{2\Delta_i} \int_0^1 dy \frac{f(y)}{y - \frac{W_i - 1}{\Delta_i}}$$

Note that

$$W_i \geq 0$$

Case I:

$$W_i < 1$$

$$y - \frac{W_i - 1}{\Delta_i} < 0$$

for all $\Delta_i > 0$ and $0 \leq y \leq 1$. In this case the integrand is never singular, the value of the integral is positive.

Case II:

$$1 \leq W_i \leq \Delta_i + 1$$

For each such W_β there is a y_j such that $y_j = \frac{W_i-1}{\Delta_i}$ for all $\Delta_i > 0$ and $0 \leq y \leq 1$. Thus the integrand has a simple pole at $y = y_j = \frac{W_i-1}{\Delta_i}$

Case III:

$$W_i > \Delta_i + 1$$

$$y - \frac{W_i - 1}{\Delta_i} < 0$$

for all $\Delta_i > 0$ and $0 \leq y \leq 1$. In this case the integrand is never singular, the value of the integral is negative.

In Case II, defining f(y) by

$$f(y) = \frac{1}{2\Delta_i} \; y^{s-1/2} \; \frac{1}{1 - \frac{Cy}{(\Delta^2+y)^6}} \cdot \frac{1}{(\Delta^2+y)^\sigma} \quad ,$$

we use the following construction to evaluate the P_i's:

$$P_i(s,\sigma) = PV \int_o^1 dy \; \frac{f(y)}{y - \frac{W_i-1}{\Delta_i}}$$

$$= f(\frac{W_i-1}{\Delta_i}) \ell n[\frac{\frac{W_i-1}{\Delta_i}}{1 - \frac{W_i-1}{\Delta_i}}] + \int_o^1 \frac{f(y)-f\frac{W_i-1}{\Delta_i}}{y - \frac{W_i-1}{\Delta_i}} \qquad (68)$$

Now, using f(y) just introduced

$$D_i(s,\sigma) = \Delta_i \int_o^1 dy f(y) \delta[\beta i(\Delta_i y+1+1-W_i)]$$

$$= \frac{1}{\beta_i} \int_o^1 dy f(y) \delta(y - \frac{W_i-1}{\Delta_i})$$

so that

$$D_i(s,\sigma) = \frac{1}{\beta_i} \; f(\frac{W_i-1}{\Delta_i}) \qquad 0 \leq \frac{W_i-1}{\Delta_i} \leq 1 \qquad (69)$$

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

All the necessary ingredients for determination of plasmon energies and lifetimes have now been assembled.

The root of the plasmon dispersion relation, eq. (30), was determined numerically by Mueller's iteration scheme[28] and the integrals in eq. (67a,b) were performed numerically using a 32 point Gauss's quadrature formula[28]. Band gaps and widths were taken from experiments where available and from band calculations or estimates when necessary. Table II in Appendix B contains all data used.

The parameter δ (see eq. (54)) was determined by requiring that eq. (30) at $\nu = 0$ gives the optical dielectric constant. Mueller's iteration scheme was again used. All calculations were performed on the IBM 360/65 computer. The results are presented in Table I. In every case listed the lifetimes are infinite.

2. Discussion and Conclusions

The reported experimental uncertainties of plasmon energies as measured in characteristic energy loss spectra[36] are on the order of 0.1 eV. However, as noted by Pines[13,29], the results of different experimenters often differ by more than this (~1 eV) thus adding to the uncertainty of the reported values. Furthermore, the band widths used are generally claimed to be within $\pm$ .2 eV of the correct value. It would thus appear that the numerical agreement of the present calculations with experiment is reasonable in both Fry's model and the "simplest approximation" of Chapter II. The results for RbCl, RbBr, and KBr show both excellent agreement with experiment and a positive shift from the free plasmon value as predicted by Wilson. This is attributed to the relatively flat, nearly degenerate valence bands throughout the

TABLE I

Calculated and Experimental Plasmon Energies (in eV)

Solid	Experimental*	Free Electron Gas	Fry's Model	Horie's Result (Modified) eq.
CsCl	11.8	12.5	13.3	12.8
KCl	13.9	13.3	13.5	14.5
NaCl	15.5	15.7	15.6	16.7
RbCl	13.9	12.4	14.0	13.9
LiBr	15.7	16.3	16.1	15.7
NaBr	14.3	14.4	14.1	14.6
RbBr	12.3	11.6	12.6	12.5
KBr	13.5	12.3	13.3	13.2
MgO	22.5	24.3	20.6	20.4
Si	16.6	16.6	18.0	17.9
MnS		17.5	21.5	
A		16.6	19.7	20.1

* Ref. (25 and 25a)

Bz and a k^2-like conduction band from Γ to L points where the conduction band width is smallest. That is, both Wilson's two-band model and Fry's model is expected to work well for such band structure. For NaCl, LiBr, NaBr, and MgO however, both the experimental and calculated shift from the free plasmon value is opposite to the prediction of Wilson. We attribute this to the non-degeneracy of the valence bands (except at Γ), thus invalidating a two-band model. Furthermore, the crossing of conduction bands along Δ lines occurs closer to the Bz face at x than in the first cases so that use of the band widths at x should be appropriate here, thus accounting for the good results. We would have expected KCl to belong in this latter group; however, its plasmon energy shift is positive. This can only be attributed to the relative size of the band widths, i.e., .04 and .1 (at L), compared to, e.g., .2 and .4 for LiBr (at X) (see Table II) which allows application of a two-band model. In the case of Si, the correct shift is obtained but the agreement with experiment is not very good. This may be due to the extreme lack of isotropy especially for the conduction bands. Furthermore, the x and y valence bands differ greatly in energy along Σ lines contrary to the assumption of Fry's model. In CsCl we find the x and y valence bands are non-degenerate over the major portion of the Bz thus accounting for the negative shift and error in the results using Fry's model.

The plasmon dispersion function, eq. (30) as calculated using Fry's model, is sketched and discussed for a few typical cases in Appendix C, in the small $\vec{q}$ limit.

Improvements over the present calculations (using Fry's model in pair approximation without local field effects) should, of course, result with the inclusion of more bands, in particular, a low-lying second conduction band for the alkali halides. Calculational difficulties appear to arise, however, when one attempts to include s-like core bands[16]. Extension of the present model to the case of metals appears straightforward but somewhat less appropriate in general on account of the fact that most metal fermi surfaces are far from spherical.

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APPENDIX A

The analytic properties of the PP are found by introducing the complete set of eigenstates of the full Hamiltonian[22]. The results[1] are obtained in the standard way and are recorded here:

$$P(q,\nu) = P(q,-\nu) \qquad \text{A-1}$$

$$P(q,\nu) = \frac{1}{\pi}\int_0^\infty d\nu' \frac{2\nu'}{(\nu'-i\eta)^2-\nu^2}\ \mathrm{Im}P(q,\nu') \qquad \text{A-2}$$

$$P(q,\nu+i\eta) = P^*(q,\nu-i\eta). \qquad \text{A-3}$$

From DuBois[20], the PP

$$P(q,\nu) = \frac{\Lambda(q,\nu)}{1 - v(q)\Lambda(q,\nu)} \qquad \text{A-4}$$

should have a pole at the plasmon energy i.e., when

$$1 - v(q)\Lambda(q,\nu) = 0 \ .$$

APPENDIX B

Band parameters are presented in Table II. In all cases experimental values for the energy gaps were available. When attempting to determine a single value for the band widths however, considerable judgment must be used as isotropy never occurs. Generally, we used the following guidelines:

(i) Use the experimental values from a single report if available. Otherwise use any combinations of experiments or experiment and calculation.

(ii) Avoid using a conduction band width which overlaps a higher conduction band when possible.

(iii) When more than two directions in k-space are given, choose a value which appears to be valid over the largest possible region of the BZ.

Cell volumes and optical dielectric constants were obtained from the standard sources[37,38,39].

TABLE II

Band Parameters Used for Calculation With Fry's Model

Solid	Band Gaps (eV)		Bandwidths (eV)					Cell Volume (A^{o3})	$\varepsilon_{optical}$	Δ
	$\beta_1 = \beta_2$ Bz Point Γ	β_3 Bz Point Γ	Bz Point	Cond + Val_{xy}	Cond + Val_z	$\Delta_1=\Delta_2$	Δ_3	Ω/N		δ/k_B
CsCl(a)	8.0	8.0	R	1.3	1.4	.163	.175	69.43	2.70	1.92
KCl(b,g)	8.69	8.81	L	.3	.9	.036	.102	61.98	2.13	2.03
NaCl(c)	8.97	9.16	X	1.9	2.4	.210	.265	44.58	2.25	2.00
RbCl(d)	8.3	8.3	L	1.9	2.0	.229	.240	69.93	2.23	1.98
LiBr(d)	7.6	7.6	X	1.4	3.0	.184	.395	41.36	3.20	1.87
NaBr(d)	7.0	7.0	X	2.2	3.5	.314	.500	52.95	2.60	1.95
RbBr(d)	7.2	7.2	L	1.6	1.7	.222	.236	80.50	2.41	1.97
KBr(b)	7.5	7.5	L	1.8	2.0	.240	.267	71.42	2.43	1.96
MgO(b,e)	7.8	7.8	X	5.6	8.2	.716	1.06	18.56	2.95	1.91
Si(f)	1.0	1.0	-	4.6	11.4	4.6	11.4	40.75	11.0	1.68
MnS(f)	6.2	6.2	-	4.0	4.0	.645	.645	35.19	6.8	1.68
A(f)	13.3	13.3	-	2.9	3.3	.218	.248	37.04	1.70	2.09

a. Reference (30) c. Reference (32) e. Reference (34) g. Reference (35)
b. Reference (31 d. Reference (33) f. Reference (16)

APPENDIX C

In figures 2 and 3 are presented the frequency dependent dispersion function $1 - v(q)\Lambda^r(q,\nu)$ for NaCl and MgO respectively. The three peaks shown occur at the band gap, the band gap plus xy valence band width and the band gap plus z valence bandwidth. At $\nu = 0$ the dispersion function has its optical value and as $\nu \to \infty$ it approaches 1. The plasmon root occurs as $1 - v(q)\Lambda^r(q,\nu)$ goes from - to +. $\Lambda^r(\vec{q},\nu)$ is calculated in the small $\vec{q}$ limit using eq. (65).

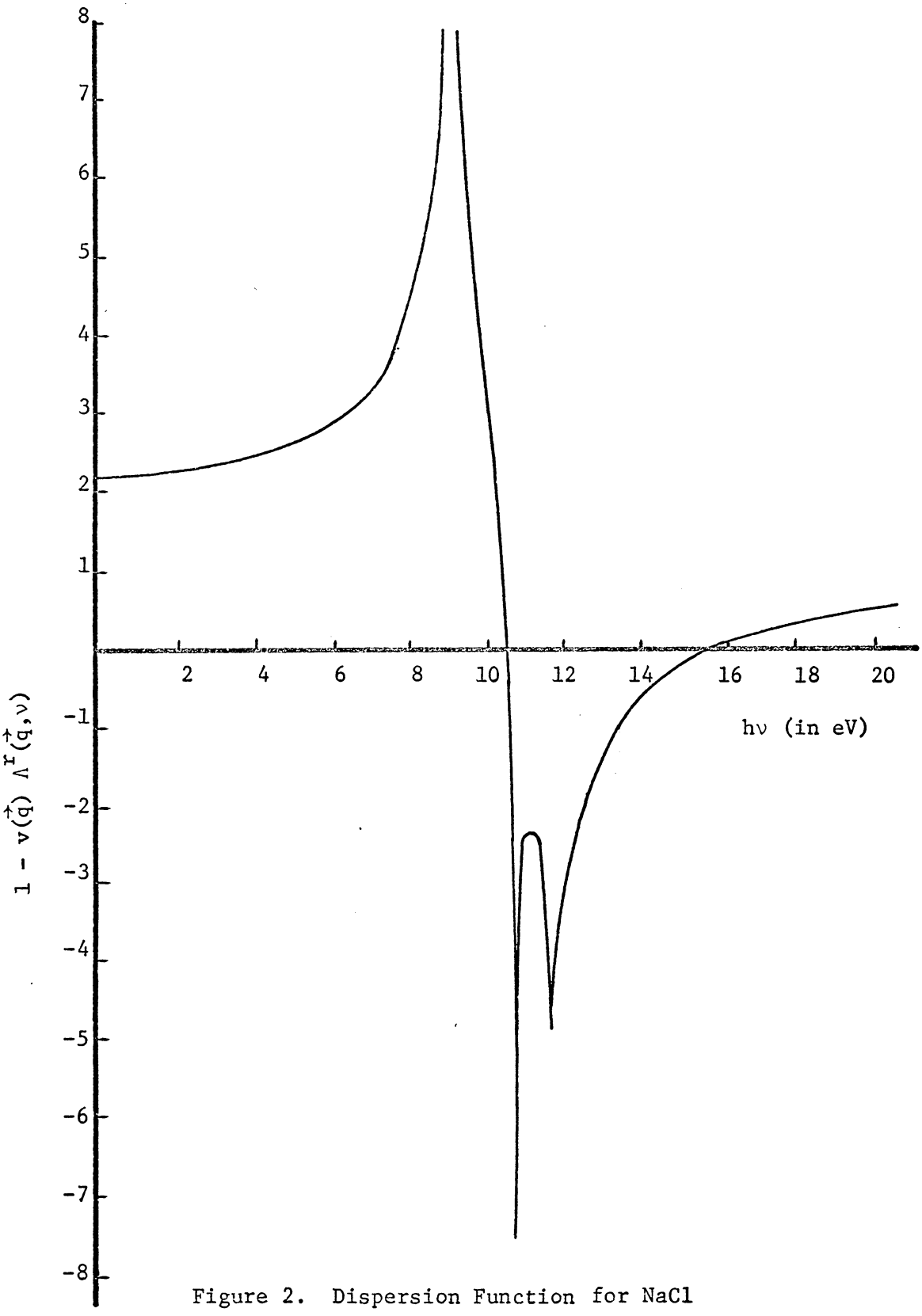

Figure 2. Dispersion Function for NaCl

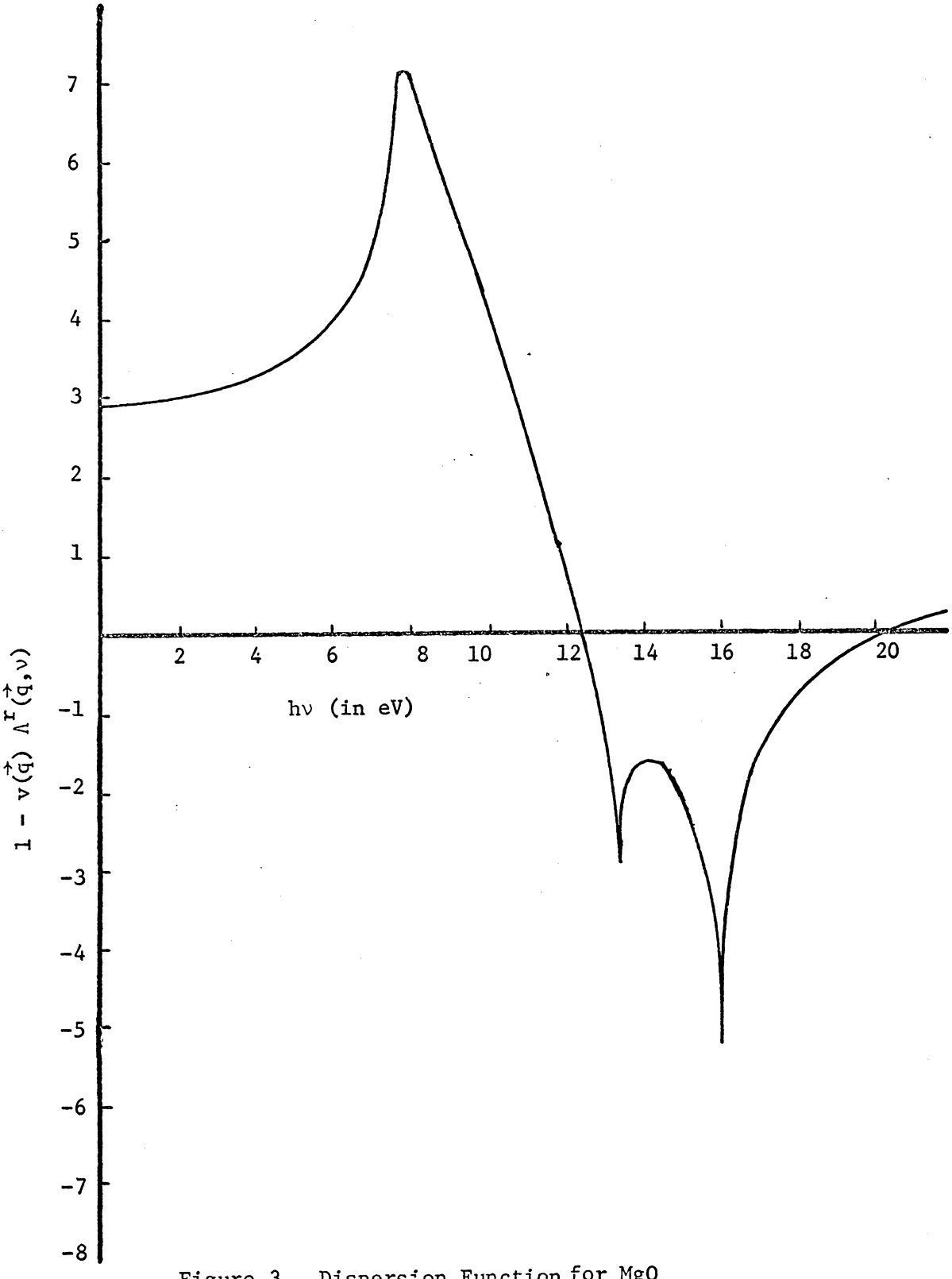

Figure 3. Dispersion Function for MgO

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GROUND STATE PERTURBATION THEORY FOR THE MANY ELECTRON SYSTEM IN A STATIC LATTICE: SOME PLASMON PROPERTIES OF INSULATORS

Chester L. Foster, Jr.

ABSTRACT

The problem of an interacting electron gas in a static lattice (an inhomogeneous electron gas) at zero temperature is treated by use of field theoretic perturbation theory. The unperturbed system is taken to be a non-interacting electron gas in a static lattice. The electron-electron interactions are then treated as a perturbation on this system. One-particle basis functions, Bloch functions, are introduced explicitly into the perturbation series for the Green functions, and diagrams associated with the various terms are defined. Certain formal results in integral equation form are noted. Using the method of DuBois, the plasmon excited state is studied. In particular, plasmon energies and lifetimes are calculated in the pair approximation for several insulators.