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CONTRIBUTION OF NEUTRAL ATOMS TO THE ABSORPTION OF PHOTONS IN PLASMAS

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ABSTRACT

In this thesis we have obtained the index of refraction and the attenuation coefficient per unit time, as well as per unit length, for an arbitrary medium using Maxwell's wave theory, and expressed the results in terms of the microscopic currents due to the motion of the particles in the medium. In Maxwell's theory, the effect of the medium is characterized by a conductivity tensor which relates the macroscopic current to the electric field. The conductivity tensor is obtained quite generally by using Kubo's linear response theory in terms of the microscopic currents.

The index of refraction and the attenuation coefficient per unit time associated with the decay of EM waves in time for weakly absorbing media has been found to be the same as those obtained by using the photon transport theory. However, the index of refraction and the attenuation coefficient per unit length associated with the decay of EM waves in space are different from those obtained by the transport theory even for weakly absorbing media.

We have also investigated in this thesis the contribution of the neutral atoms to the absorption of photons in plasmas, by extending the Akcasu and Wald's work on the absorption due to the inverse bremsstrahlung of electrons in the field of neutral atoms to higher electron temperatures and higher photon energies, and formulated this problem by using plane waves for electron wave function. In this way we have obtained an expression for the absorption coefficient per unit length due to the above absorption mechanism in terms of the elastic and inelastic electron-atom scattering cross sections allowing the atoms initially to be in any excited state. We have calculated the absorption coefficient explicitly for hydrogen atoms, and presented the results graphically as a function of electron temperature and radiation frequency. Using these curves and the conventional formula for the absorption due to the photoionization and its inverse, we have computed the net total absorption due to the neutral atoms numerically, and compared our results to the absorption measured by Litvak and Edwards. In estimating the distribution of the neutral atoms, as well as the size of the plasma produced by the laser pulse in their experiment, we have used the point explosion theory with spherical shock wave. The agreement between the calculated and measured absorptions has been found to be better than a factor of 10 and in fact better than a factor of 6 in all, but one, initial gas pressures (The observed discrepancies may be attributed mainly to the use of the radius of the peak luminous volume, which is assumed to be shperical, as the actual shock wave radius).

In the absence of any accurate information for the plasma size, and of an explosion theory which takes into account the finite initial volume of the explosion caused by the laser beam, the agreement obtained is considered as a strong evidence for the importance of neutral atoms in certain absorption

experiments in plasmas over ions, because the absorption calculated by considering the electron inverse bremsstrahlung in the field of ions only is about 100 times less than the observed values.

CHAPTER I

INTRODUCTION

This thesis contains primarily an investigation of low-energy photon absorption in an arbitrary medium. At low photon energies, the pair production and annihilation processes are negligible and scattering is characterized by the Thomson cross section rather than Compton cross section. In stellar systems, the Thompson scattering may be important, but in laboratory plasmas it is usually negligible because of its small cross section. Thus our analysis in this thesis is restricted to the systems in which the scattering is negligible, and the net photon absorption is primarily due to bremsstrahlung and inverse bremsstrahlung, ionization and recombination, and excitation and deexcitation.

The equations of radiative transfer for dispersive and nondispersive media are usually developed by phenomenological consideration.[1-4] A systematic, self-contained derivation of a photon transport equation for nondispersive media from fundamental consideration was made in 1961 by Osborn and Klevans.[5] In their derivation, a photon distribution function in analogy with the quantum mechanical distribution function for particles[6] was introduced. The equation they obtained can be reduced to the conventional radiative transfer equation obtained phenomenologically for nondispersive media.

A year later, they extended their theory to dispersive media[7] by making use of the concept of "dressed photon" first introduced by Mead.[8]

A "dressed photon" has a different frequency ω_k in the medium than the free space value ck, but it has the same wave length in the medium and in free space. With the "dressed photon" technique they derived, in the framework of the first order perturbation theory, a photon transport equation for dispersive media. This equation differs from the radiative transfer equation obtained phenomenologically in dispersive media by others.(3,4) In order to compare these two theories, Wald(9) performed an experiment in 1966 in which he measured the absorption of microwave radiation in slightly ionized helium. Although a better agreement is obtained by the photon transport equation than the radiative transfer equation in his measurement, conclusive evidence of the validity of the photon transport equation or the invalidity of the radiative transfer equation cannot be inferred from his measurement because the refractive defocussing effects are not neglibible.

Since the net photon absorption and the refractive index in dispersive media can be easily deduced from the photon transport equation, the validity of this equation can be tested if the net photon absorption and the refractive index can be obtained independently by an entirely different approach. Such an approach to the calculation of the net photon absorption and the refractive index can be achieved by using Kubo's theory(10) for electric conductivity and the Maxwell equations. In this approach, the absorption coefficient and the index of refraction are expressed in terms of the microscopic current due to motion of all particles in the medium. To facilitate the comparison we obtain in section II-1 the net photon absorption and the refractive index using the photon transport equation also in terms of the microscopic current. The expected value of electric current is obtained from Kubo's theory in section II-2. Using the expected value of the current in the Maxwell equation (II-40), a dispersion relation between the wave vector $\underline{k}$, the frequency ω, and the electric conductivity can be obtained. Two different sets of results for photon absorption and refractive index in weakly absorbing media are obtained by considering the damping of the electromagnetic wave in time and in space. A comparison of the results obtained from these two theories is presented in section II-3.

In order to display the various mechanisms contributing to the photon absorption and also to estimate the order of magnitude of the various contributions, we use a convenient and simple representation for the particle system in Chapter III. Second quantization is used to express the various potentials between particles, as well as the interactions between particle and radiation, in terms of the particle and radiation creation and destruction operators. Starting from the golden rule, one can obtain, with several approximations discussed in section II-2, a simple expression which displays the various mechanisms contributing to the photon absorption, such as the bound-bound transition, bremsstrahlung of electrons in the fields of the neutrals and ions, the induced dipole transitions, etc. At the end of this chapter we give a simple and crude investigation of the variation of photon absorption with time after the formation of a plasma. This investigation is motivated by the absorption measurements, being performed now in The University of Michigan, in which a continuous He-Ne laser beam (6328Å) is incident on the decaying plasma produced by exploding lithium wire. The validity of this simple investigation could not be verified because the measurements have not reached the final stage yet.

In Chapter IV, we will be concerned with the radiation absorption only due to inverse bremsstrahlung of electrons moving in the field of neutral atoms at high gas temperatures (~ 20 eV). The same problem at low gas temperatures (~ 1 eV or less) was investigated in 1960 by Firsov and Chibisov(11) and recently extended by Akcasu and Wald.(12) At low temperatures, the electron energies are insufficient to excite an atom from its ground state to an excited state. Assuming that all the atoms in the system are initially and finally in the ground state, they calculated the various absorption contributions due to neutral-inverse bremsstrahlung, induced dipole transition, and exchange and interference effects by partial wave method and found that the last three contributions for low temperature system are negligible as compared to the first one.

An experiment measuring the absorption coefficient for the ruby laser beam (6943Å) in a hydrogen plasma produced by a giant pulsed laser beam was carried out in 1966 by Litvak and Edwards.(13) Their calculated absorption coefficient obtained by considering photoionization and inverse bremsstrahlung of electrons in the field of ions is two orders of magnitude less than their measured result. Chapter IV is motivated primarily by this large discrepancy.

The temperature of the plasma in Litvak and Edwards experiment is high ($\theta \sim 20$ eV). Most of the hydrogen atoms are found in excited states and the energies of electrons are sufficient to excite the atoms from a level to a higher level. The electron-atom scattering cross section increases when the atom is in an excited state. As seen from Akcasu and Wald's work, this cross section enters in the expression for radiation absorption. Since at high temperatures, an appreciable number of hydrogen atoms are in upper levels and the above cross section at these levels is high, one may expect the neutral bremsstrahlung to be a dominant process contributing to the radiation absorption in Litvak and Edwards' experiment. This is one reason for extending in Chapter IV the calculations by Akcasu and Wald to high temperatures. The other reason is that the total number density of hydrogen atoms in different states, determined in the case of Litvak and Edwards' experiment by the initial gas conditions with the assumption of ideal gas, is ten or more times the electron (or ion) density depending upon the initial gas pressure.

In the formulation of the problem, we use the second order perturbation theory in which electron states are represented by plane waves. In this approximation, the electron-hydrogen cross section is calculated in the first Born approximation. Although a more accurate result is expected by using partial waves, the use of free electron wave function makes the problem more manageable.

If all the atoms in the system are initially and finally in the ground state, as assumed by Akcasu and Wald, with the assumption that the cross section involved is slowly varying up to the incident energy of electrons, we obtain the same result as obtained by Akcasu and Wald through the partial wave method (section IV-2).

An application of the above theoretical results to hydrogen plasma is presented in sections IV-3, IV-4, and IV-5. In order to explain the measured absorptions in Litvak and Edwards experiment by considering the photoionization process and the inverse bremsstrahlung of electrons in the field of neutral atoms, we use in section IV-7 the point explosion theory in estimating the number density of neutral atoms in the plasma produced by the laser beam. The comparison between our calculated absorptions and the measured results are discussed in section IV-8.

CHAPTER II

PHOTON ABSORPTION AND REFRACTIVE INDEX

In this chapter we shall present two different approaches to the calculation of photon absorption and refractive index in an arbitrary particle system. The first approach is based on photon transport theory developed by Osborn and Klevans,[5,7] the second one, on Kubo's theory[10] of electric conductivity. The comparison between the results from these two theories will be made at the end of this chapter.

1. PHOTON TRANSPORT THEORY

In 1961, Osborn and Klevans[5] used first order perturbation theory in developing photon transport for nondispersive media, and a year later they[7] extended the theory to dispersive media by making use of the concept of "dressed photon" first introduced by Mead.[8] In this section we shall use their results for dispersive media to express the photon absorption and the refractive index in terms of the microscopic current due to motion of all particles in the medium. This requires, in the first place, a description of the hamiltonian of the particle system, the radiation field, and the interaction between these two, as well as the introduction of the concept of "dressed photon."

Consider a box of volume L^3 in the particle system under consideration. The hamiltonian for the particles in this volume element interacting with a radiation field can be written in the nonrelativistic theory as

$$H = H^R + \sum_\sigma \left[\sum_j \frac{\{\underline{p}_{\sigma j} - \frac{e_{\sigma j}}{c} \underline{A}(\underline{r}_{\sigma j})\}^2}{2m_{\sigma j}} + V_\sigma \right] + V' = H_o + H^{PR} \qquad \text{(II-1)}$$

with

$$H_o = H^R + H^P \qquad \text{(II-2)}$$

$$H^{PR} = H^{PR1} + H^{PR2} \qquad \text{(II-3)}$$

where

$$H^P = \sum_\sigma \left[\sum_j \frac{\underline{p}^2_{\sigma j}}{2m_{\sigma j}} + V_\sigma \right] + V' \qquad \text{(II-4)}$$

$$H^{PR1} = - \sum_{\sigma j} \frac{e_{\sigma j}}{2m_{\sigma j}c} \{\underline{p}_{\sigma j} \cdot \underline{A}(\underline{r}_{\sigma j}) + \underline{A}(\underline{r}_{\sigma j}) \cdot \underline{p}_{\sigma j}\} \qquad \text{(II-5)}$$

$$H^{PR2} = \sum_{\sigma j} \frac{e^2_{\sigma j}}{2m_{\sigma j}c^2} \underline{A}^2(\underline{r}_{\sigma j}) \qquad \text{(II-6)}$$

In the above equations, H^R and $\underline{A}(r)$ are, respectively, the hamiltonian and the vector potential of the radiation field. The symbols $m_{\sigma j}$, $e_{\sigma j}$, $\underline{p}_{\sigma j}$, and $\underline{r}_{\sigma j}$ denote the mass, charge, momentum, and position of the j-th particle in the σ-th molecule. Here, we use the term "molecule" in a general sense to refer to any aggregate of particles bound together. The number of constituent particles in a molecule is arbitrary. It proves to be convenient to regard even an electron as a simple molecule as defined above. V_σ is the potential between the particles in the σ-th molecule and V' is the potential between the molecules in L^3.

Interactions between particles in different boxes via long-range coulomb forces constitute a small effect upon photon-particle interactions within a box and we may expect that neglect of this effect produces negligible error. Then the photo-particle interaction of the system can be approximated as the sum of the interactions in each box.

The customary procedure[14] requires that the (transverse) radiation field be periodic at the boundaries of a normalization box whose volume is assumed here to be L^3. The vector potential of the field at a point $\underline{r}$ can then be represented by operators in the Schrödinger picture as

$$\underline{A}(\underline{r}) = \sum_{\lambda\underline{k}} \sqrt{\frac{2\pi\hbar c}{L^3 k}}\, e^{-i\underline{k}\cdot\underline{r}} \{\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k}) + \alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\} \qquad \text{(II-7)}$$

and the hamiltonian of the radiation field turns to be

$$H^R = \sum_{\lambda\underline{k}} \frac{1}{2}\hbar\, ck\, \{\alpha_\lambda^\dagger(\underline{k})\alpha_\lambda(\underline{k}) + \alpha_\lambda(\underline{k})\alpha_\lambda^\dagger(\underline{k})\} \qquad \text{(II-8)}$$

where $\alpha_\lambda^\dagger(\underline{k})$ and $\alpha_\lambda(\underline{k})$ are creation and destruction operators for photons of momentum $\hbar\underline{k}$ and polarization λ in free space. $\underline{\epsilon}_\lambda(\underline{k})$ is a unit polarization vector. The creation and destruction operators satisfy the commutation relations

$$[\alpha_\lambda(\underline{k}),\ \alpha_{\lambda'}(\underline{k}')] = [\alpha_\lambda^\dagger(\underline{k}),\ \alpha_{\lambda'}^\dagger(\underline{k}')] = 0$$

$$[\alpha_\lambda(\underline{k}),\ \alpha_{\lambda'}^\dagger(\underline{k}')] = \delta_{\lambda\lambda'}\delta_{\underline{k}\underline{k}'} \qquad \text{(II-9)}$$

Since the radiation is in constant interaction with the medium, Mead introduced the concept of "dressed photon" by associating photons in the medium with a different frequency ω_k than the free space value ck, keeping the wavelengths in medium and in free space the same. In doing this, he used a different expansion of $\underline{A}(\underline{r})$ due originally to Bohm and Pines[15] and showed that the creation and destruction operators $a_\lambda^\dagger(\underline{k})$ and $a_\lambda(\underline{k})$ for creating and destructing photons of frequency ω_k are different from the free space operators $\alpha_\lambda^\dagger(\underline{k})$ and $\alpha_\lambda(\underline{k})$. They are related through the relationship

$$a_\lambda(\underline{k}) = \frac{1}{2}\left(\frac{\omega_k}{ck}\right)^{\frac{1}{2}} \{(1+\frac{ck}{\omega_k})\alpha_\lambda(\underline{k})+(1-\frac{ck}{\omega_k})\alpha_\lambda^\dagger(-k)\}$$

$$a_\lambda^\dagger(\underline{k}) = \frac{1}{2}\left(\frac{\omega_k}{ck}\right)^{\frac{1}{2}} \{(1-\frac{ck}{\omega_k})\alpha_\lambda(-\underline{k})+(1+\frac{ck}{\omega_k})\alpha_\lambda^\dagger(k)\} \qquad \text{(II-10)}$$

or

$$\alpha_\lambda(\underline{k}) = \frac{1}{2(\omega_k ck)^{\frac{1}{2}}}\{(ck+\omega_k)a_\lambda(\underline{k})+(ck-\omega_k)a_\lambda^\dagger(-\underline{k})\}$$

$$\alpha_\lambda^\dagger(\underline{k}) = \frac{1}{2(\omega_k ck)^{\frac{1}{2}}}\{(ck+\omega_k)a_\lambda^\dagger(\underline{k})+(ck-\omega_k)a_\lambda(-\underline{k})\} \ . \qquad \text{(II-11)}$$

It is clear that $\alpha_\lambda(\underline{k})$ and $a_\lambda(\underline{k})$ become identical when $\omega_k = ck$. It can be verified easily that $a_\lambda(\underline{k})$ and $a_\lambda^\dagger(\underline{k})$ satisfy the same commutation relations as $\alpha_\lambda(\underline{k})$ and $\alpha_\lambda^\dagger(\underline{k})$ even with $\omega_k \neq ck$.

The substitution of eqs. (II-11) into eqs. (II-6), (II-7), and (II-8), i.e., expressing H^{PR2}, $\underline{A}(\underline{r})$, and H^R in terms of the operators $a_\lambda^\dagger(\underline{k})$ and $a_\lambda(\underline{k})$, gives

$$\underline{A}(r) = \sum_{\lambda\underline{k}}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_k}}e^{-i\underline{k}\cdot\underline{r}} \{a_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+a_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\} \qquad \text{(II-12)}$$

$$H^R = H^{R0} + H^{R1} + H^{R2} \qquad \text{(II-13)}$$

$$H^{PR2} = H_o^{PR2} + H_1^{PR2} + H_2^{PR2} \qquad \text{(II-14)}$$

where

$$H^{R0} = \sum_{\lambda\underline{k}}\frac{\hbar\omega_k}{2}\{a_\lambda^\dagger(\underline{k})a_\lambda(\underline{k})+a_\lambda(\underline{k})a_\lambda^\dagger(\underline{k})\} \qquad \text{(II-15)}$$

$$H^{R1} = \sum_{\lambda\underline{k}}\frac{\hbar}{4}\frac{c^2k^2-\omega_k^2}{\omega_k}\{a_\lambda^\dagger(\underline{k})a_\lambda(\underline{k})+a_\lambda(\underline{k})a_\lambda^\dagger(\underline{k})\} \qquad \text{(II-16)}$$

$$H^{R2} = \sum_{\lambda\underline{k}}\frac{\hbar}{4}\frac{c^2k^2-\omega_k^2}{\omega_k}\{a_\lambda^\dagger(\underline{k})a_\lambda^\dagger(-\underline{k})+a_\lambda(\underline{k})a_\lambda(-\underline{k})\} \qquad \text{(II-17)}$$

$$H_o^{PR2} = \sum_{\sigma j\lambda\underline{k}}\frac{\pi\hbar e_{\sigma j}^2}{L^3 m_{\sigma j}\omega_k}\{a_\lambda^\dagger(\underline{k})a_\lambda(\underline{k})+a_\lambda(\underline{k})a_\lambda^\dagger(\underline{k})\} \qquad \text{(II-18)}$$

$$H_1^{PR2} = \sum_{\sigma j\lambda k} \frac{\pi\hbar e_{\sigma j}^2}{L^3 m_{\sigma j}\omega_k} \{a_\lambda^\dagger(\underline{k})a_\lambda^\dagger(-\underline{k})+a_\lambda(-\underline{k})a_\lambda(\underline{k})\} \tag{II-19}$$

$$H_2^{PR2} = \sum'_{\lambda\underline{k}\lambda'\underline{k}'} \sum_{\sigma j} \frac{\pi\hbar\, e_{\sigma j}^2}{L^3 m_{\sigma j}} \frac{e^{-i(\underline{k}-\underline{k}')\cdot\underline{r}_{\sigma j}}}{(\omega_k\omega_{k'})^{\frac{1}{2}}} \{a_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+a_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\}$$

$$\cdot\{a_{\lambda'}^\dagger(-\underline{k}')\underline{\epsilon}_{\lambda'}(-\underline{k}')+a_{\lambda'}(\underline{k}')\underline{\epsilon}_{\lambda'}(\underline{k}')\} \tag{II-20}$$

$$\sum'_{\lambda\underline{k}\lambda'\underline{k}'} \text{ means } \sum_{\lambda k\neq\lambda' k'} .$$

Then the hamiltonian for the whole system (particles in L^3 plus radiation) can be written, in terms of the operators $a_\lambda^\dagger(k)$ and $a_\lambda(k)$, as $H=H_o'+H^I$ with $H_o' = H^{RO}+H^P$ and $H^I=H^{PR1}+(H^{R1}+H_o^{PR2})+(H^{R2}+H_1^{PR2})+H_2^{PR2}$ where

$$H^{RI} + H_o^{PR2} = \frac{\hbar}{4}\sum_{\lambda k}\left\{\sum_{\sigma j}\frac{4\pi e_{\sigma j}^2}{L^3 m_{\sigma j}\omega_k} + \frac{c^2k^2-\omega_k^2}{\omega_k}\right\}\{a_\lambda^\dagger(\underline{k})a_\lambda(\underline{k})+a_\lambda(\underline{k})a_\lambda^\dagger(\underline{k})\} \tag{II-21}$$

$$H^{R2} + H_1^{PR2} = \frac{\hbar}{4}\sum_{\lambda k}\left\{\sum_{\sigma j}\frac{4\pi e_{\sigma j}^2}{L^3 m_{\sigma j}\omega_k} + \frac{c^2k^2-\omega_k^2}{\omega_k}\right\}\{a_\lambda^\dagger(k)a_\lambda^\dagger(-k)+a_\lambda(k)a_\lambda(-k)\} \tag{II-22}$$

In obtaining the photon transport equation and refractive index, Klevans[7] formulated the problem in the representation in which the particle state $|n>$ and the photon state $|\eta>$ satisfy

$$H^P|n> = E_n|n> \quad H^{RO}|\eta> = E_\eta|\eta>$$

i.e., (II-23)

$$H_o'|n\eta> = E_{n\eta}|n\eta>,\ E_{n\eta} = E_n+E_\eta$$

With H^I regarded as the perturbed hamiltonian. The obtained photon transport equation is given by

$$\frac{\partial f_\lambda(\underline{r},\underline{k},t)}{\partial t} + \underline{\Omega}\cdot\nabla v f_\lambda(\underline{r},\underline{k},t) = \sum_{n\eta,n'\eta'} \{\eta_\lambda'(\underline{k})-\eta_\lambda(\underline{k})\} \Gamma_{n'\eta',n\eta} D_{n\eta,n\eta} \quad \text{(II-24)}$$

where $f_\lambda(\underline{r},\underline{k},t)$ is the expected number of photons with momentum $\hbar\underline{k}$ and polarization λ in the volume L^3 located at the point $\underline{r}$. The photons are moving with the velocity $v\underline{\Omega}$ in the direction of the unit vector $\underline{\Omega}$. v is different for dispersive media from the speed of light c. $\Gamma_{n'\eta',n\eta}$ is the transition probability from the initial state $|n\eta>$ to the final state $|n'\eta'>$ which is given, in first order perturbation theory, by

$$\Gamma_{n'\eta',n\eta} \approx \frac{2\pi}{\hbar} |<n'\eta'|H^I|n\eta>|^2 \delta(E_{n'\eta'}-E_{n\eta}). \quad \text{(II-25)}$$

$\eta_\lambda(\underline{k})$ is the occupation number of photons with $\hbar\underline{k}$ and λ, and D is the density operator of the whole system (particles and radiation).

In addition to the photon transport equation, the refractive index of the medium can also be obtained by letting

$$\sum_{n\eta} D_{n\eta,n\eta}(S_{n\eta}-S_{no}) = o \quad \text{(II-26)}$$

where $S_{n\eta}$ is the shift of the energy level $E_{n\eta}$ for the state $|n\eta>$ and given by

$$S_{n\eta} = <n\eta|H^I|n\eta> + \sum_{n'\eta'\neq n\eta} P \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} \quad \text{(II-27)}$$

where P indicates the principal value. S_{no} is a shift of the self-energy of the medium when no photons are present and can be obtained by letting η=o in eq. (II-27).

With the above results, we shall express the photon absorption coefficient and the refractive index of the medium in terms of the microscopic current due to motion of all particles in L^3 in the following two sections.

a. Photon Absorption Coefficient

The processes involved in obtaining the photon absorption coefficient are single photon emission and absorption. The only contribution to these processes comes from H^{PR1} because H^{R1}, H_o^{PR2}, H^{R2}, H_1^{PR2}, and H_2^{PR2} are bilinear in photon operators. Define the current operator due to motion of all the particles in L^3 as

$$\underline{J}(\underline{r}) = \sum_{\sigma j} \frac{e_{\sigma j}}{2m_{\sigma j}} \{\underline{p}_{\sigma j}\delta(\underline{r}-\underline{r}_{\sigma j})+\delta(\underline{r}-\underline{r}_{\sigma j})\underline{p}_{\sigma j}\}, \tag{II-28}$$

then

$$H^{PR1} = - \int d^3r\, \underline{J}(\underline{r}) \cdot \frac{\underline{\underline{A}}(\underline{r})}{c} \tag{II-29}$$

where the integration takes over the volume L^3. From eqs. (II-23) and the definition of Dirac δ-function

$$\delta(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{\frac{ixt}{\hbar}}\, dt, \tag{II-30}$$

the substitution of eqs. (II-29) and (II-25) into eq. (II-24) gives

$$\frac{\partial f_\lambda(\underline{r},\underline{k},t)}{\partial t} + \underline{\Omega} \cdot \nabla v f_\lambda(\underline{r},\underline{k},t) = Q_\lambda(\underline{r},\underline{k},t)$$

where

$$Q_\lambda(\underline{r},\underline{k},t) = \sum_{n\eta} \frac{D_{n\eta,n\eta}}{\hbar^2} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \,\Big\{ \sum_{n'} \langle n|\underline{J}(\underline{r})|n'\rangle \cdot \langle\eta|\frac{\underline{\underline{A}}(\underline{r})}{c}|\eta+1\rangle$$

$$\otimes\langle\eta+1|\frac{\underline{\underline{A}}(\underline{r}',t')}{c}|\eta\rangle \cdot \langle n'|\underline{J}(\underline{r}',t')|n\rangle - \sum_{n''} \langle n|\underline{J}(\underline{r})|n''\rangle \cdot \langle\eta|\frac{\underline{\underline{A}}(\underline{r})}{c}|\eta-1\rangle$$

$$\otimes\langle\eta-1|\frac{\underline{\underline{A}}(\underline{r}',t')}{c}|\eta\rangle \cdot \langle n''|\underline{J}(\underline{r}',t')|n\rangle \Big\} \tag{II-31}$$

with

$$\underline{J}(\underline{r},t) = e^{\frac{i}{\hbar}H^P t}\, \underline{J}(\underline{r}) e^{-\frac{i}{\hbar}H^P t} \tag{II-32}$$

$$\underline{A}(r,t) = e^{\frac{i}{\hbar}H^{RO}t}\,\underline{A}(\underline{r})e^{-\frac{i}{\hbar}H^{RO}t} \qquad \text{(II-33)}$$

being the Heisenberg operators. The first sum in the bracket of eq. (II-31) comes from photon emission by letting $\eta'=\eta+1$ in eq. (II-24). The second term comes from photon absorption by letting $\eta'=\eta-1$.

Evaluating the matrix elements of $\underline{A}(\underline{r})$ and $\underline{A}(\underline{r},t)$ in Eq. (II-31) by use of eqs. (II-12) and (II-33), and suming the intermediate states $|n'\rangle$ and $|n''\rangle$, one obtains

$$Q_\lambda(\underline{r},\underline{k},t) = \sum_{n\eta} \frac{2\pi D_{n\eta,n\eta}}{L^3\hbar\omega_k} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \langle n|J_\lambda(\underline{r})J_\lambda(\underline{r}',t')|n\rangle$$

$$\times\left\{ e^{i\omega_k t'} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \sqrt{\eta_\lambda(\underline{r},\underline{k})+1}\sqrt{\eta_\lambda(\underline{r}',\underline{k})+1} - e^{-i\omega_k t'} e^{-i\underline{k}\cdot(\underline{r}-\underline{r}')} \sqrt{\eta_\lambda(\underline{r},\underline{k})\eta_\lambda(\underline{r}',\underline{k})} \right\}$$

where

$$J_\lambda(\underline{r},t) = \underline{J}(\underline{r},t)\cdot\underline{\epsilon}_\lambda(\underline{k}).$$

At this stage we introduce several approximations which enable us to reduce $Q_\lambda(\underline{r},\underline{k},t)$ to a simple form. The first approximation is to replace $D_{n\eta,n\eta}$ by $D^P_{nn}\,D^R_{\eta\eta}$. D^P is the density operator of the medium only and given by $D^P=e^{-\beta H^P}/Tre^{-\beta H^P}$ with $\beta=\frac{1}{\Theta}$ being the reciprocal of the medium temperature in the units of energy. D^R is the density operator of the radiation field and given by $D^R=e^{-\beta H^{RO}}/Tre^{-\beta H^{RO}}$. This approximation implies that the particle system and the radiation field are initially statistically independent and permits us to perform the statistical averages over the particle and photon states separately. The second approximation is equivalent to replacing the average of a function by the function of the average in performing the statistical average of the factor containing the photon occupation number, i.e.,

$$\sum_\eta D^R_{\eta\eta} \sqrt{1+\eta_\lambda(\underline{r},\underline{k})}\sqrt{1+\eta_\lambda(\underline{r}',\underline{k})} \approx \sqrt{1+f_\lambda(\underline{r},k)}\sqrt{1+f_\lambda(\underline{r}',k)}.$$

With these two approximations, $Q_\lambda(\underline{r},\underline{k},t)$ reduces to

$$Q_\lambda(\underline{r},\underline{k},t) = \frac{2\pi}{L^3\hbar\omega_k}\int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \Big\{ e^{i\omega_k t'} e^{ik\cdot(\underline{r}-\underline{r}')}\sqrt{1+f_\lambda(\underline{r},\underline{k})}\sqrt{1+f_\lambda(\underline{r}',\underline{k})}$$

$$-e^{-i\omega_k t'} e^{-i\underline{k}\cdot(\underline{r}-\underline{r}')}\sqrt{f_\lambda(\underline{r},\underline{k})f_\lambda(\underline{r}',\underline{k})}\Big\} \mathrm{Tr}D^P J_\lambda(\underline{r})\, J_\lambda(\underline{r}',t')$$

We recall that integrations over $\underline{r}$ and $\underline{r}'$ are extended to the same box of volume L^3. If we further assume that $f_\lambda(\underline{r},\underline{k})$ is slowly varying over the box volume then we can take the product of the square roots outside the integral. Interchanging $\underline{r}$ and $\underline{r}'$ and letting $t'=-t'$ in the second term, one finally obtains, by using the property TrABC=TrBCA,

$$\frac{\partial}{\partial t} f_\lambda(\underline{r},\underline{k},t) + \underline{\Omega}\cdot Dvf_\lambda(\underline{r},\underline{k},t) = -\alpha^t_\lambda(\underline{k},\omega_k)f_\lambda(\underline{r},\underline{k},t) + E_\lambda(\underline{k},\omega_k) \quad \text{(II-33)}$$

where

$$\alpha^t_\lambda(\underline{k},\omega_k) = \frac{2\pi}{L^3\hbar\omega_k}\int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' e^{-i\omega_k t'} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}\, \mathrm{Tr}D^P[J_\lambda(\underline{r}',t'),J_\lambda(\underline{r})] \quad \text{(II-34a)}$$

$$E_\lambda(\underline{k},\omega_k) = \frac{2\pi}{L^3\hbar\omega_k}\int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' e^{i\omega_k t'} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}\, \mathrm{Tr}D^P\, J_\lambda(\underline{r})J_\lambda(\underline{r}',t') \quad \text{(II-35)}$$

are respectively the net absorption coefficient and the spontaneous emission coefficient per unit time for photons of momentum $\hbar\underline{k}$ and polarization λ. In an infinite homogeneous medium, $\mathrm{Tr}D^P[J_\lambda(\underline{r}',t'),J_\lambda(\underline{r})]$ can depend only on the difference of the positions $\underline{r}-\underline{r}'$. In a large finite system, this translational invariance will be approximately true in regions away from boundaries. One of the integrations over the position can be performed. Then

$$\alpha_\lambda^t(\underline{k},\omega_k) = \frac{2\pi}{\hbar\omega_k} \int d^3r' \int_{-\infty}^{\infty} dt' e^{i\omega_k t'} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \mathrm{Tr} D^P [J_\lambda(\underline{r}',t'), J_\lambda(\underline{r})] \quad \text{(II-34)}$$

In view of eq. (II-33) it is obvious that the photon absorption coefficient per unit length is given by

$$\alpha_\lambda^s(\underline{k},\omega_k) = \frac{\alpha_\lambda^t(\underline{k},\omega_k)}{v} . \quad \text{(II-36)}$$

In a later section we shall compare eqs. (II-34) and (II-36) to the expressions for photon absorption obtained by Kubo's theory. The superscripts s and t over the absorption coefficients per unit length and per unit time, respectively, are introduced here to facilitate this comparison.

b. Index of Refraction

We mentioned before that the index of refraction in dispersive media can be obtained by letting $\sum_{n\eta} D_{n\eta,n\eta}(S_{n\eta}-S_{no})=o$. From eq. (II-27),

$$\sum_{n\eta} D_{n\eta,n\eta}(S_{n\eta}-S_{no}) = \sum_{n\eta} D_{n\eta,n\eta}\Bigg[\langle n\eta|H^I|n\eta\rangle - \langle no|H^I|no\rangle + \sum_{n'\eta'\neq n\eta} P \frac{|\langle n'\eta'|H^I|n\eta\rangle|^2}{E_{n\eta}-E_{n'\eta'}} - \sum_{n'\eta'\neq no} P \frac{|\langle n'\eta'|H^I|no\rangle|^2}{E_{no}-E_{n'\eta'}}\Bigg] \quad \text{(II-37)}$$

Recalling H^I and Eqs. (II-5), (II-20), (II-21), and (II-22), it is readily established that

$$\langle n\eta|H^I|n\eta\rangle = \langle n\eta|H^{R1}+H_o^{PR2}|n\eta\rangle = \sum_{\lambda\underline{k}} \frac{\hbar}{4}\left\{\sum_{sj}\frac{4\pi N_s e_{sj}^2}{L^3 m_{sj}\omega_k} + \frac{c^2k^2-\omega_k^2}{\omega_k}\right\}(2\eta_\lambda(\underline{k})+1) \quad \text{(II-38)}$$

and

$$\langle no|H^I|no\rangle = \langle no|H^{R1}+H_o^{PR2}|no\rangle = \sum_{\lambda\underline{k}} \frac{\hbar}{4}\left[\sum_{sj}\frac{4\pi N_s e_{sj}^2}{L^3 m_{sj}\omega_k} + \frac{c^2k^2-\omega_k^2}{\omega_k}\right] \quad \text{(II-39)}$$

where N_s is the number of the molecules of kind S in L^3 and e_{sj} and m_{sj}

are the charge and mass of the jth particle in a molecule of kind S.

Note that $<n'\eta|H^I|n\eta> = <n'o|H^I|no> = o$ for $n' \neq n$, and $<n\eta'|H^I|n\eta> = o$ for $\eta' = \eta \pm 1$ and for $\eta = o$, $\eta' = 1$, then one obtains

$$\sum_{n'\eta' \neq n\eta} \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} = \sum_{n' \neq n} \frac{|<n'\eta|H^I|n\eta>|^2}{E_n - E_{n'}} + \sum_{\eta' \neq \eta} \frac{|<n\eta'|H^I|n\eta>|^2}{E_\eta - E_{\eta'}}$$

$$+ \sum_{\substack{n' \neq n \\ \eta' \neq \eta}} \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} = \sum_{\substack{n' \neq n \\ \eta' \neq \eta}} \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} \qquad \text{(II-40)}$$

and

$$\sum_{n'\eta' \neq no} \frac{|<n'\eta'|H^I|no>|^2}{E_{no}-E_{n'\eta'}} = \sum_{\substack{n' \neq n \\ \eta' \neq o}} \frac{|<n'\eta'|H^I|no>|^2}{E_{no}-E_{n'\eta'}} \, . \qquad \text{(II-41)}$$

Using the property of Dirac δ-function $f(E)= \int_{-\infty}^{\infty} f(x)\delta(x-E)dx$, eqs. (II-40) and (II-41) become

$$\sum_{n'\eta' \neq n\eta} \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} = \sum_{\substack{n' \neq n \\ \eta' \neq \eta}} \int_{-\infty}^{\infty} d\omega' \frac{|<n'\eta'|H^{PR1}|n\eta>|^2}{\hbar\omega'} \delta(\omega' - \frac{E_{n\eta}-E_{n'\eta'}}{\hbar})$$

and

$$\sum_{n'\eta' \neq no} \frac{|<n'\eta'|H^I|no>|^2}{E_{no}-E_{n'\eta'}} = \sum_{\substack{n' \neq n \\ \eta' \neq \eta}} \int_{-\infty}^{\infty} d\omega' \frac{|<n'\eta'|H^{PR1}|no>|^2}{\hbar\omega'} \delta(\omega' - \frac{E_{no}-E_{n'\eta'}}{\hbar}) \, .$$

The substitution of eq. (II-29) and the use of eq. (II-30) gives, after a straightforward manipulation (see Appendix A),

$$\sum_{n'\eta' \neq n\eta} \frac{|<n'\eta'|H^I|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} - \sum_{n'\eta' \neq no} \frac{|<n'\eta'|H^I|no>|^2}{E_{no}-E_{n'\eta'}}$$

$$= - \sum_{\lambda \underline{k}} \frac{\eta_\lambda(\underline{k})}{L^3 \omega_k} \int d^3r \int d^3r' \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} dt' \frac{e^{i\omega' t'}}{\omega' - \omega_k} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}$$

$$\times <n|J_\lambda(\underline{r}')J_\lambda(\underline{r},-t')-J_\lambda(\underline{r})J_\lambda(\underline{r}',t')|n> \, . \qquad \text{(II-42)}$$

By taking the statistical average over the photon state $|\eta>$ as in the case of absorption coefficient, using TrABC=TrBCA and substituting eqs. (II-38), (II-39), and (II-42) into eq. (II-37), one obtains

$$\sum_{\lambda k}\frac{\hbar\omega_k}{2}f_\lambda(\underline{r},\underline{k})\left\{\frac{\sum_{sj}\frac{4\pi N_s e_{sj}^2}{L^3 m_{sj}}+c^2k^2-\omega_k^2}{\omega_k^2}\right.$$

$$\left.-\frac{2}{L^3\hbar\omega_k^2}\int d^3r\int d^3r'\int_{-\infty}^{\infty}dt\ P\int_{-\infty}^{\infty}d\omega'\ \frac{e^{i\omega't'}}{\omega'-\omega_k}e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}\mathrm{Tr}D^p\ [J_\lambda(\underline{r}';t'),J_\lambda(\underline{r})]\right\}=0.$$

Then the refractive index for dispersive media is obtained, in terms of the microscopic current due to motion of all the particles in L^3, as

$$n_0^2 = \left(\frac{ck}{\omega_k}\right)^2 = 1+\frac{4\pi b_\lambda(\underline{k},\omega_k)}{\omega_k} \qquad \text{(II-43)}$$

where

$$b_\lambda(\underline{k},\omega_k) = \frac{1}{2\pi\hbar\omega_k}\int d^3r'\int_{-\infty}^{\infty}dt'\,P\int_{-\infty}^{\infty}d\omega'\ \frac{e^{i\omega't'}}{\omega'-\omega_k}e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}\mathrm{Tr}D^p[J_\lambda(\underline{r}';t'),J_\lambda(\underline{r})]\ -\frac{q^2}{\omega_k} \qquad \text{(II-44)}$$

$$q^2 = \sum_{sj}\frac{N_s}{L^3}\frac{e_{sj}^2}{m_{sj}} \qquad \text{(II-45)}$$

and the property that $\mathrm{Tr}D^p[J_\lambda(\underline{r}';t'),J_\lambda(\underline{r})]$ can depend only on $\underline{r}-\underline{r}'$ for an infinite homogeneous medium has been used. In section II-3, we shall compare eqs. (II-34), (II-36), and (II-43) with the results obtained from Kubo's theory.

2. KUBO'S THEORY

In 1957, Kubo[(10)] developed the theory of linear response of a medium to an external field (i.e., electromagnetic waves) acting on the medium. He showed that the response can be described by electric conductivity tensor of the medium. In 1966 Dong[16] applied the theory to fully-ionized plasmas. In this section we shall use Kubo's theory to obtain the photon (or radiation) absorption coefficient and the refractive index for an arbitrary, electrically neutral medium which may be a neutral gas, or partially or full-ionized plasma.

From Maxwell's equations, one can obtain

$$\nabla^2 \underline{E}(\underline{r},t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\underline{E}(\underline{r},t) = \frac{4\pi}{c^2}\frac{\partial}{\partial t}\underline{J}^e(\underline{r},t) \qquad \text{(II-46)}$$

by assuming that the macroscopic charge density of the medium is zero, i.e.,

$$\underline{\nabla}\cdot\underline{E}(\underline{r},t) = o.$$

Thus $\underline{E}(\underline{r},t)$ is transverse. We used the superscript e over $\underline{J}(\underline{r},t)$ in eq. (II-46) to denote that it is the expected value of the current operator $\underline{J}(\underline{r},t)$. By using the gauge in which the scalar potential vanishes, the electric field $\underline{E}(\underline{r},t)$ can be described by a vector potential $\underline{A}(\underline{r},t)$ through the relationship

$$\underline{E}(\underline{r},t) = -\frac{1}{c}\frac{\partial}{\partial t}\underline{A}(\underline{r},t). \qquad \text{(II-47)}$$

Assume that the external field turns on at $t=-\infty$. Before the field is imposed on the medium, we have

$$[D^p,\ H^p] = o.$$

At time t, the interaction hamiltonian between the system and the applied external field can be written as

$$V(t) = -\sum_{oj}\frac{e_{oj}}{2m_{oj}c}\{\underline{p}_{oj}\cdot\underline{A}(\underline{r}_{oj},t)+\underline{A}(\underline{r}_{oj},t)\cdot\underline{p}_{oj}\} + \sum_{oj}\frac{e_{oj}^2}{2m_{oj}c^2}\underline{A}^2(\underline{r}_{oj},t)$$

$$= H_1(t)+H_2(t) \qquad \text{(II-48)}$$

where

$$H_1(t) = -\int d^3r\ \underline{J}(\underline{r}) \cdot \frac{\underline{A}(\underline{r},t)}{c} \qquad \text{(II-49)}$$

$$H_2(t) = -\frac{1}{2}\int d^3r\ \underline{J}_A(\underline{r},t) \cdot \frac{\underline{A}(\underline{r},t)}{c} \qquad \text{(II-50)}$$

$$\underline{J}_A(\underline{r},t) = -\sum_{oj} \frac{e_{oj}^2}{m_{oj}c}\, \delta(\underline{r}-\underline{r}_{oj})\underline{A}(\underline{r}_{oj},t) \qquad \text{(II-51)}$$

With $\underline{J}(\underline{r})$ defined as eq. (II-28). When the medium is acted upon by the field $\underline{A}(\underline{r},t)$, the total current operator at the time t becomes

$$\underline{J}(\underline{r},t) = \underline{J}(\underline{r}) + \underline{J}_A(\underline{r},t).$$

The expected value of $\underline{J}(\underline{r},t)$ is defined by

$$\underline{J}^e(\underline{r},t) = Tr[\underline{J}(\underline{r}) + \underline{J}_A(\underline{r},t)]D(t) \qquad \text{(II-52)}$$

where D(t) is the density operator of the perturbed system at time t and satisfies the Liouville equation

$$\frac{d}{dt} D(t) = \frac{i}{\hbar}\,[D(t),\ H^p + H_1(t) + H_2(t)] \qquad \text{(II-53)}$$

with the boundary condition $D(t=-\infty) = D^p$.

For a weak perturbation, we shall obtain the current response $J_\ell^e(\underline{r},t)$ to first order in $\underline{A}$. For this purpose we substitute

$$D(t) = D^p + D_1(t) \qquad \text{(II-54)}$$

into eq. (II-53) where $D_1(t)$ is the perturbation due to $\underline{A}$ and neglect the terms $[D^p, H_2(t)]$ and $[D_1(t), H_1(t)+H_2(t)]$ in the resulting equation (note that H_1 is first order and H_2 is second order in $\underline{A}$). Then, D_1 satisfies

$$\frac{d}{dt} D_1(t) = \frac{i}{\hbar}\,[D_1(t),\ H^p] + \frac{i}{\hbar}\,[D^p, H_1(t)] \qquad \text{(II-55)}$$

whose solution is readily found as

$$D_1(t) = \frac{i}{\hbar}\int_{-\infty}^{t} dt' \left[D^p, e^{-\frac{i}{\hbar}H^p(t-t')} H_1(t') e^{\frac{i}{\hbar}H^p(t-t')}\right]. \qquad \text{(II-56)}$$

The substitution of eqs. (II-54) and (II-56) into eq. (II-52) gives, after neglecting the terms containing $\underline{A}^2(\underline{r},t)$,

$$J^e_\ell(\underline{r},t) = \mathrm{Tr}D^p J_\ell(\underline{r}) + \mathrm{Tr}D^p J_{A\ell}(\underline{r},t)$$

$$+ \frac{i}{\hbar} \int d^3r' \int_{-\infty}^{t} dt' \; \mathrm{Tr}D^p \, [J_\ell(\underline{r},t), \; J_m(\underline{r}',t')] \, \frac{A_m(\underline{r}',t')}{c} \qquad \text{(II-57)}$$

where the subscripts ℓ and $m(\ell, m=1,2,3)$ refer to the components of the vectors and where the summation convention on the repeated indices is used. The first term in eq. (II-57) is the expected value of the current in the unperturbed medium and is zero. The second term is given explicitly by

$$\mathrm{Tr}D^p \underline{J}_A(\underline{r},t) = - \sum_n D^p_{nn} \langle n | \sum_{\sigma j} \frac{e^2_{\sigma j}}{m_{\sigma j} c} \, \delta(\underline{r}-\underline{r}_{\sigma j}) \underline{A}(\underline{r}_{\sigma j},t) | n \rangle \, .$$

Since the delta function is contained in the matrix element, the integration over all the coordinates of particles will give

$$\mathrm{Tr}D^p \underline{J}_A(\underline{r},t) = -q^2 \, \frac{\underline{A}(\underline{r},t)}{c} \qquad \text{(II-58)}$$

where q^2 is defined in eq. (II-45). Then eq. (II-57) becomes

$$J^e_\ell(\underline{r},t) = -q^2 \, \frac{A_\ell(\underline{r},t)}{c} + \frac{i}{\hbar} \int d^3r' \int_{-\infty}^{t} dt' \; \mathrm{Tr}D^p [J_\ell(\underline{r},t), \; J_m(\underline{r}',t')] \, \frac{A_m(\underline{r}',t')}{c} \, . \qquad \text{(II-59)}$$

In order to calculate the absorption and refractive index in the framework of Kubo's theory, we substitute eq. (II-59) into eq. (II-46) and use eq. (II-47) to eliminate the vector potential in favor of the electric field. The result is

$$\nabla^2 E_\ell(\underline{r},t) - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} E_\ell(\underline{r},t) = \frac{4\pi}{c^2} \int d^3r' \int_{-\infty}^{t} dt' \{ q^2 \delta(t-t') \delta(\underline{r}-\underline{r}') \delta_{\ell m}$$

$$- \frac{i}{\hbar} \mathrm{Tr} D^p [J_\ell(\underline{r}, t-t'), J_m(\underline{r}')] E_m(\underline{r}', t') \qquad \text{(II-60)}$$

or

$$\nabla^2 \underline{E}(\underline{r}, t) - \frac{1}{c^2} \frac{\partial}{\partial t^2} \underline{E}(\underline{r}, t) = \frac{4\pi}{c^2} \int d^3r' \int_{-\infty}^{t} dt' \underline{\underline{\sigma}}(\underline{r}-\underline{r}', t-t') \cdot \underline{E}(\underline{r}', t') \qquad \text{(II-61)}$$

where $\underline{\underline{\sigma}}(\underline{R}, \tau)$ is called the conductivity tensor. We shall give the explicit form of $\underline{\underline{\sigma}}$ in the transformed domain later.

Equation (II-60) which describes the electric field in the medium can be solved if one specifies the boundary and the initial conditions on $\underline{E}(\underline{r}, t)$. The solution can in general be constructed in terms of the solution of the homogeneous equation of the following form

$$\underline{\epsilon}_\lambda e^{-(i\underline{k}\cdot\underline{r} - i\omega t)} \qquad \text{(II-62)}$$

where $\underline{k}$ and ω are related to each other through the dispersive relation.

$$k^2 - \frac{\omega^2}{c^2} = - \frac{4\pi i\omega}{c^2} \sigma_\lambda(\underline{k}, \omega) \qquad \text{(II-63)}$$

where $\sigma_\lambda(\underline{k}, \omega)$ is the scalar conductivity defined by

$$\sigma_\lambda(\underline{k}, \omega) = \underline{\epsilon}_\lambda \cdot \underline{\underline{\sigma}}(\underline{k}, \omega) \cdot \underline{\epsilon}_\lambda$$

where $\underline{\underline{\sigma}}(\underline{k}, \omega)$ is the transform of $\underline{\underline{\sigma}}(\underline{R}, \tau)$ and explicitly given by

$$\sigma_\lambda(\underline{k}, \omega) = - \frac{iq^2}{\omega} - \frac{1}{\hbar\omega} \int d^3r' \int_0^\infty d\tau e^{-i\omega\tau} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \mathrm{Tr} D^p [J_\lambda(\underline{r}, \tau), \underline{J}_\lambda(\underline{r}')] \qquad \text{(II-64)}$$

In the applications, one usually encounters two types of problem: (1) initial value problem and (2) boundary value problem. In the first case, one specifies an initial spatial distribution $\underline{E}(\underline{r}, o)$ and solves for $\underline{E}(\underline{r}, t)$ for $t > o$. The initial distribution can be expressed as superposition of the terms of spatial modes of the helmholtz operator, i.e., $e^{i\underline{k}\cdot\underline{r}}$ where $\underline{k}$ is real vector. The damping associated with each mode is obtained by solving the dispersion relation as $\omega(k)$ for a given real k.

In the second type of problem, one solves the Maxwell's equation (II-60) for $\underline{E}(\underline{r},t)$ when $\underline{E}(\underline{r},t)$ is specified on the boundary as a known function of time. The time dependence can be expressed as the superposition of terms of the form $e^{i\omega t}$ where ω is a real number. The associated complex $\underline{k}$ is obtained from the dispersion relation as $\underline{k}(\omega)$. A sinusoidal plane wave impinging on the side of an half infinite medium is a typical example for problems of the second kind. The complex number $\underline{k}(\omega)$ in this case is the inverse relaxation length in the medium.

We shall compare the Kubo theory to transport theory in these two typical cases.

a. Damping in Time

As we mentioned above, we must solve the dispersion relation in this case for a real $\underline{k}$, and obtain the real and imaginary parts of $\omega(\underline{k})$ for a given $\underline{k}$. It is convenient to substitute

$$\omega = \frac{\omega_o}{n(\underline{k})} = \frac{\omega_o}{n_o + i n_1} \qquad \text{(II-65)}$$

where $\omega_o = ck$, and $n(\underline{k})$ is called the complex refractive index with n_o and n_1 as its real and imaginary parts. The electric field will decay in time as $e^{-2\omega_I t}$ where ω_I is the imaginary part of $\omega(\underline{k})$. $2\omega_I$ is the decay rate of the electric field which is the quantity to be compared to the photon absorption coefficient per unit time $\alpha^t_\lambda(\underline{k},\omega_k)$ obtained in photon transport theory.

The substitution of eq. (II-65) into the dispersion relation eq. (II-63) gives

$$1-\frac{n_o^2-n_1^2}{(n_o^2+n_1^2)^2}+i\frac{2n_on_1}{(n_o^2+n_1^2)^2}=-\frac{4\pi i}{\omega_o(n_o+in_1)}\sigma_\lambda(\underline{k},\frac{\omega_o}{n_o+in_1})$$

In order to solve the dispersion relation for the real and imaginary parts of $\omega(\underline{k})$, we shall consider a weakly absorbing medium, $n_1 \ll n_o$. In this case the dispersion relation can be approximated as

$$1-\frac{1}{n_o^2}+i\frac{2n_1}{n_o^3}=-\frac{4\pi i}{n_o^2\omega_k}\{\sigma_\lambda^R(\underline{k},\omega_k)+i\,\sigma_\lambda^I(\underline{k},\omega_k)\}$$

where $\omega_k=\frac{\omega_o}{n_o}$ is exactly the frequency used in photon transport theory and $\sigma_\lambda^R(\underline{k},\omega_k)$ and $\sigma_\lambda^I(\underline{k},\omega_k)$ are respectively the real and imaginary parts of the scalar conductivity $\sigma_\lambda(\underline{k},\omega_k)$ given by eq. (II-64).

Equating the real and imaginary parts, one obtains the real refractive index

$$n_o^2=1+\frac{4\pi}{\omega_k}\sigma_\lambda^I(\underline{k},\omega_k)\ , \qquad \text{(II-66)}$$

the imaginary part

$$n_1=-\frac{2\pi n_o}{\omega_k}\sigma_\lambda^R(\underline{k},\omega_k)$$

and the decay rate of the electric field

$$2\omega_I=-\frac{2n_1\omega_k}{n_o}=4\pi\sigma_\lambda^R(\underline{k},\omega_k). \qquad \text{(II-67)}$$

The explicit form of $\sigma_\lambda(\underline{k},\omega)$ was given in eq. (II-64) for complex ω. When $\omega=\frac{\omega_o}{n_o}=\omega_k$, we have

$$\sigma_\lambda(\underline{k},\omega_k)=-\frac{iq^2}{\omega_k}-\frac{1}{\hbar\omega_k}\int d^3r'\int_0^\infty d\tau e^{-i\omega_k\tau}e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}\mathrm{Tr}D^p[J_\lambda(\underline{r},\tau),\ J_\lambda(\underline{r}')]$$

By using the integration representation of the unit step function, i.e.,

$$U(\tau) = \frac{i}{2\pi} \int_{-\infty}^{\infty} ds \, \frac{e^{-is\tau}}{s+i\epsilon} \quad \text{with } \epsilon \to 0$$

and letting $\tau = -t'$ and $\omega' = s+\omega_k$, then

$$i\sigma_\lambda(\underline{k},\omega_k) = \frac{q^2}{\omega_k} + \frac{1}{2\pi\omega_k\hbar} \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega' \, \frac{e^{i\omega' t'}}{\omega'-\omega_k+i\epsilon} \, e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \mathrm{Tr} D^p [J_\lambda(\underline{r}), J_\lambda(\underline{r}';t')].$$

The real and imaginary parts of $\sigma_\lambda(k,\omega_k)$ can be obtained by noting that

$$\lim_{\epsilon \to 0} \frac{1}{\omega'-\omega+i\epsilon} = P\frac{1}{\omega'-\omega} - i\pi\delta(\omega'-\omega)$$

as

$$\sigma_\lambda^R(\underline{k},\omega_k) = \frac{1}{2\hbar\omega_k} \int d^3r' \int_{-\infty}^{\infty} dt' e^{i\omega_k t'} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \mathrm{Tr} D^p [J_\lambda(\underline{r}';t'), J_\lambda(\underline{r})] \qquad \text{(II-68)}$$

$$\sigma_\lambda^I(\underline{k},\omega_k) = \frac{1}{2\pi\hbar\omega_k} \int d^3r' \int_{-\infty}^{\infty} dt' \, P\int_{-\infty}^{\infty} d\omega' \, \frac{e^{i\omega' t'}}{\omega'-\omega_k} \, e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \mathrm{Tr} D^p [J_\lambda(\underline{r}';t'), J_\lambda(\underline{r})] - \frac{q^2}{\omega_k} \qquad \text{(II-69)}$$

b. Damping in Space

As mentioned above, the dispersion relation must be solved in this case for a real $\omega = \omega_o$ to obtain the real and imaginary parts of $\underline{K}(\omega_o)$. It is convenient to let

$$\underline{K} = (n_o + in_1)\underline{k}$$

where $ck = \omega_o$. For a weakly absorbing medium $n_1 \ll n_o$, the dispersion relation eq. (II-63) can be approximated as

$$n_o^2 - 1 + 2in_1 n_o = -\frac{4\pi i}{\omega_o} \{\sigma_\lambda^R(n_o\underline{k},\omega_o) + i\sigma_\lambda^I(n_o\underline{k},\omega_o)\}.$$

Then, the real refractive index and the imaginary part are

$$n_o^2 = 1 + \frac{4\pi\sigma_\lambda^I(n_o\underline{k},\omega_o)}{\omega_o} \qquad \text{(II-70)}$$

and

$$n_1 = -\frac{2\pi}{n_o\omega_o}\,\sigma_\lambda{}^R(n_o\underline{k},\omega_o)\ . \qquad \text{(II-71)}$$

The E.M. wave absorption per unit length is

$$\alpha_\lambda(\underline{k},\omega_o) = -2n_1 k = \frac{4\pi}{n_o c}\,\sigma_\lambda{}^R(n_o\underline{k},\omega_o). \qquad \text{(II-72)}$$

This is the quantity to be compared to the photon absorption coefficient per unit length $\alpha_\lambda^S(\underline{k},\omega_k)$ obtained in photon transport theory.

In eqs. (II-70), (II-71), and (II-72), $\sigma_\lambda{}^R(n_o\underline{k},\omega_o)$ and $\sigma_\lambda{}^I(n_o\underline{k},\omega_o)$ have the exact forms as eqs. (II-68) and (II-69) except that the places where k and ω_k occupy are respectively replaced by $n_o\underline{k}$ and ω_o.

3. Comparison of the Results From Two Theories

The resulting expression obtained by substituting eq. (II-68) into eq. (II-67) is identical to eq. (II-34), and, furthermore, eq. (II-66) with the substitution of eq. (II-69) is the same as eq. (II-43) with the substitution of eq. (II-44). One can conclude that the photon absorption coefficient per unit time and the refractive index obtained from photon transport theory are the same as that obtained from Kubo's theory through damping in time only for weakly absorbing media. Since eqs. (II-36) and (II-43) are not the same as eqs. (II-72) and (II-70), respectively, the photon absorption coefficient per unit length and the refractive index obtained in the former theory are different than that obtained in the latter theory through damping in space even for a weakly absorbing medium.

As mentioned in section II-1, the "dressed photon" concept used in photon transport theory is to associate photons in medium with the same wavelength $\lambda = \frac{2\pi}{k}$ as in free space, but a different frequency ω_k from ck. It is obvious that the dressed photon technique is equivalent to damping E.M. wave in time because the latter is to consider E.M. wave in medium as a wave having the same wavelength as, but a different frequency from the free space values. It is different from damping E.M. wave in space because the latter is to regard E.M. wave in medium having the same frequency as, but a different wavelength from the free space values.

From the above conclusions and reasons, it seems suggestive to formulate photon transport theory by associating photons in medium with the same frequency as, but a different wave number vector from that in free space. Then the photon absorption coefficient per unit length and the refractive index obtained from such formulated photon transport theory may turn out the same results as obtained from Kubo's theory by damping E.M. wave in space. It would not give the photon absorption coefficient per unit time and the refractive index as obtained from Kubo's theory by damping E.M. wave in time. However, the suggested formulation is more desirable because most measurements have been usually done in measuring photon absorption coefficient per unit length.

CHAPTER III

VARIOUS PHOTON ABSORPTION MECHANISMS

In chapter II, we have obtained the absorption coefficient for a photon with momentum $\hbar\underline{k}$ and polarization λ in dispersive media. We shall restrict ourselves, henceforth, to a nondispersive medium. In order to display various mechanisms contributing to the photon absorption in a material medium and also to estimate the order of magnitudes of the various contributions in the lowest approximation we shall change the representation $\{|n\rangle\}$ for the description of the particle system. In chapter II, the particle wave functions $|n\rangle$ were chosen as the eigenfunctions of the total hamiltonian

$$H^p = \sum_\sigma \left[\sum_j \frac{\underline{p}_{\sigma j}^2}{2m_{\sigma j}} + V_\sigma \right] + V'$$

which included the interaction between various constituent molecules. In the present chapter we shall work with a representation which diagonalizes only part of H^p. The remaining part of H^p will be treated as perturbation.

1. DESCRIPTION OF THE PARTICLE SYSTEM IN FIRST ORDER PERTURBATION APPROXIMATION

For a particle system which consists of neutral atoms, singly-charged ions and free electrons, the hamiltonian of the system can be written as

$$H^p = H^A + H^i + H^e + V^p$$

$$V^p = V^{AA} + V^{ee} + V^{ii} + V^{Ae} + V^{Ai} + V^{ie}$$

where H^A, H^i, and H^e are, respectively, the hamiltonians of the neutral atoms, the singly-charged ions and the free electrons. V^{AA}, V^{ee} and V^{ii} are the potentials between the same kind of "molecules" (atoms, ions and free electrons), and V^{Ae}, V^{Ai}, and V^{ie} are the potentials between the different kind of "molecules."

In addition to H^p, the interaction of the particles with the radiation field can be separated as

$$H^{pRl} = V_A + V_e + V_i$$

where V_A, V_e, and V_i are, respectively, the interactions of the atoms, the free electrons, and the ions with the radiation field.

A convenient and simple representation which one can choose is that the wave functions $|n\rangle = |\alpha\beta\gamma\rangle$ satisfy separately the Schrödinger equations

$$H^A|\alpha\rangle = E_\alpha|\alpha\rangle$$

$$H^e|\beta\rangle = E_\beta|\beta\rangle$$

$$H^i|\gamma\rangle = E_\gamma|\gamma\rangle$$

with $V=V^p + H^{pRl}$ considered as the perturbed hamiltonian. Since each of H^A, H^e, and H^i can be separated as the sum of the hamiltonians for the molecules of the same kind, the wave function $|\alpha\beta\gamma\rangle$ is the product of the wave functions for the individual molecules in the system. In this representation we must calculate the transition probabilities at least to the second order in V if we want to investigate absorption due to free-free transitions of charged particles. The photon transport equation then becomes

$$\frac{\partial}{\partial t} f_\lambda(\underline{r},\underline{k},t) + \underline{\Omega}\cdot\underline{\nabla} f_\lambda(\underline{r},\underline{k},t) = \sum_{\substack{n\eta \\ n'\eta'}} \frac{2\pi D_{n\eta,n\eta}}{\hbar} (\eta'-\eta) | \langle n'\eta'|V|n\eta\rangle$$

$$+ \sum_{\substack{n''\eta'' \\ \neq n\eta, n'\eta'}} \frac{\langle n'\eta'|V|n''\eta''\rangle\langle n''\eta''|V|n\eta\rangle}{E_{n\eta}-E_{n'\eta'}} |^2 \delta(E_{n'\eta'}-E_{n\eta}) \qquad \text{(III-1)}$$

For the reduction of eq. (III-1), we shall use second quantization in which the potentials V^{Ae}, V^{Ai}, and V^{ie} and the interactions V_A, V_e, and V_i are given by (see Appendix B)

$$V^{Ae} = \sum_{\substack{\underline{KK}' \\ aa' \\ \underline{uu}'}} \frac{4\pi e^2 \delta_K(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')}{L^3 |\underline{u}-\underline{u}'|^2} \langle a'| -z + \sum_{j=1}^{z} e^{i(\underline{u}-\underline{u}')\cdot\underline{\rho}_j} |a\rangle A^\dagger(\underline{K}'a')A^\dagger(\underline{u}')A(\underline{K}a)A(u) \qquad \text{(III-2)}$$

$$V^{Ai} = \sum_{\substack{\underline{KK}'\underline{\ell\ell}' \\ aa'bb'}} \frac{4\pi e^2 \delta_K(\underline{K}-\underline{K}'+\underline{\ell}-\underline{\ell}')}{L^3 |\underline{K}-\underline{K}'|^2} \langle a'|z-\sum_{j=1}^{z} e^{-i(\underline{K}-\underline{K}')\cdot\underline{\rho}_j}|a\rangle\langle b'|z-\sum_{j=1}^{z-1} e^{i(\underline{K}-\underline{K}')\cdot\underline{\rho}_j}|b\rangle$$

$$\times A^\dagger(\underline{K}'a')A^\dagger(\underline{\ell}'b')A(\underline{K}a)A(\underline{\ell}b) \qquad \text{(III-3)}$$

$$V^{ie} = \sum_{\substack{\underline{\ell\ell}' \\ bb' \\ \underline{uu}'}} \frac{4\pi e^2 \delta_K(\underline{\ell}-\underline{\ell}'+\underline{u}-\underline{u}')}{L^3 |\underline{u}-\underline{u}'|^2} \langle b'| -z + \sum_{j=1}^{z-1} e^{i(\underline{u}-\underline{u}')\cdot\underline{\rho}_j} |b\rangle A^\dagger(\underline{\ell}'b')A^\dagger(\underline{u}')A(\underline{\ell}b)A(\underline{u}) \qquad \text{(III-4)}$$

$$V_A = \sum_{\substack{\lambda\underline{k} \\ \underline{K}a \\ \underline{K}'a'}} \frac{ie}{c} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}} \delta_K(\underline{K}-\underline{K}'-\underline{k})\omega_{a'a}\underline{d}_{a'a} \cdot [\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})]A^\dagger(\underline{K}'a')A(\underline{K}a) \qquad \text{(III-5)}$$

$$V_e = \sum_{\substack{\lambda\underline{k} \\ \underline{uu}'}} \frac{e\hbar}{mc} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}} [\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})]\cdot\underline{u}\ \delta_K(\underline{u}-\underline{u}'-\underline{k})A^\dagger(\underline{u}')A(\underline{u}) \qquad \text{(III-6)}$$

$$V_i = \sum_{\substack{\lambda\underline{k} \\ \underline{\ell}b \\ \underline{\ell}'b'}} \frac{ie}{c} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}}\, \delta_K(\underline{\ell}-\underline{\ell}'-\underline{k})\omega_{b'b}\underline{d}_{b'b} \cdot \{\alpha_\lambda(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\}\, A^\dagger(\underline{\ell}'b')A(\underline{\ell}b) \tag{III-7}$$

where

$$\underline{d}_{a'a} = \langle a'|\sum_{j=1}^{Z}\underline{\rho}_j|a\rangle, \quad \underline{d}_{b'b} = \langle b'|\sum_{j=1}^{Z-1}\underline{\rho}_j|b\rangle, \quad \omega_{x'x} = \frac{E_{x'}-E_x}{\hbar}.$$

In the above equations, $A(\underline{u})$, $A(\underline{K}a)$, and $A(\underline{\ell}b)$ are, respectively, the destruction operators for the annihilation of a free electron of the momentum $\hbar\underline{u}$, an atom of the external (center-of-mass) momentum $\hbar\underline{K}$ and the internal state $|a\rangle$ and an ion of the external momentum $\hbar\underline{\ell}$ and the internal state $|b\rangle$. $A^\dagger(\underline{u}')$, $A^\dagger(\underline{K}'a')$, and $A^\dagger(\underline{\ell}'b')$ are the creation operators which create a free electron, an atom and an ion in different external and internal states. The symbol δ with subscript K denotes the Kronecker delta. $\underline{\rho}_j$ is the position of the j-th atomic electron in an atom or ion with respect to the position of its nucleus. $e\underline{d}_{a'a}$ (or $e\underline{d}_{b'b}$) is the matrix element of the dipole operator with respect to the internal atomic (or ion) states. $\hbar\omega_{a'a}$ (or $\hbar\omega_{b'b}$) is the energy difference of the internal states $|a'\rangle$ and $|a\rangle$ (or $|b'\rangle$ and $|b\rangle$) of an atom (or ion).

2. TRANSITION PROBABILITY FOR PHOTON EMISSION

In this section, we shall make several approximations to reduce eq. (III-1) to a simple form. The number of photons with momentum $\hbar\underline{k}$ and polarization λ emitted from L^3 per unit time can be obtained by letting $\eta'=\eta+1$ in eq. (III-1), i.e.

$$\underset{\sim}{E}_\lambda(\underline{k})(f_\lambda(\underline{k})+1) = \sum_{\substack{nn'\\ \eta}} \frac{2\pi}{\hbar} D_{n\eta,n\eta} \left| \langle n'\eta+1|V|n\eta\rangle + \sum_{\substack{n''\eta'' \\ =n\eta,n'\eta+1}} \frac{\langle n'\eta+1|V|n''\eta''\rangle\langle n''\eta''|V|n\eta\rangle}{E_{n\eta}-E_{n''\eta''}} \right|^2$$

$$\times\ \delta(E_{n'\eta+1}-E_{n\eta}) \tag{III-8}$$

where $E_\lambda(\underline{k})$ is the transition probability per unit time for emission of a photon of momentum $\hbar\underline{k}$ and polarization λ. Let us consider first the direct transition, the first term in the absolute square of eq. (III-8). Since the potential V^p between the particles contains neither the photon creation nor destruction operator, then

$$\langle n'\eta+1|V|n\eta\rangle = \langle\alpha'\eta+1|V_A|\alpha\eta\rangle\delta_{\beta\beta'}\delta_{\gamma\gamma'} + \langle\beta'\eta+1|V_e|\beta\eta\rangle\delta_{\alpha\alpha'}\delta_{\gamma\gamma'}$$

$$+ \langle\gamma'\eta+1|V_i|\gamma\eta\rangle\delta_{\alpha\alpha'}\delta_{\beta\beta'}$$

where $\langle\beta'\eta+1|V_e|\beta\eta\rangle\delta_{\alpha\alpha'}\delta_{\gamma\gamma'}$ accounts for the direct photon emission through the interaction of the free electrons with the radiation field. No such transition can exist because the energy and momentum conservation laws can not simultaneously hold (see the justification in Appendix C). Then

$$\langle n'\eta+1|V|n\eta\rangle = \langle\alpha'\eta+1|V_A|\alpha\eta\rangle\delta_{\beta\beta'}\delta_{\gamma\gamma'} + \langle\gamma'\eta+1|V_i|\gamma\eta\rangle\delta_{\alpha\alpha'}\delta_{\beta\beta'} \tag{III-9}$$

The second term in the absolute square of eq. (III-8) accounts for the indirect photon emission through the intermediate states $|n''\eta''\rangle$. It has the non-zero contribution only for $\eta''=\eta$ and $\eta''=\eta+1$.

$$\sum_{n''\eta''\neq n\eta,n'\eta+1} \frac{\langle n'\eta+1|V|n''\eta''\rangle\langle n''\eta''|V|n\eta\rangle}{E_{n\eta}-E_{n''\eta''}} = \sum_{n''\neq n'} \frac{\langle n'|V^p|n''\rangle\langle n''\eta+1|H^{PR1}|n\eta\rangle}{E_{n'}-E_{n''}}$$

$$+ \sum_{n''\neq n} \frac{\langle n'\eta+1|H^{pR1}|n''\eta\rangle\langle n''|V^p|n\rangle}{E_n-E_{n''}} \tag{III-10}$$

where we have used $E_{n'\eta+1}-E_{n\eta}=o$ from the energy conservation delta function in obtaining the demoninator of the first sum. To simplify eq. (III-10), the following three assumptions will be made throughout this chapter.

(i) The neglect of the potentials between the molecules of the same kind (i.e., neglect of V^{AA}, V^{ee}, and V^{ii}). This assumption is justified because these potentials do not affect the photon emission and absorption much, although they play an important role in the shape of the lines (pressure broadening). Under this assumption, eq. (III-10) becomes

$$\sum_{n''\eta''\neq n\eta,n'\eta+1} \frac{<n'\eta+1|V|n''\eta''><n''\eta''|V|n\eta>}{E_{n\eta}-E_{n''\eta''}}$$

$$= \sum_{\beta''}\left\{\frac{<\beta'\eta+1|Ve|\beta''\eta><\alpha'\beta''|V^{Ae}|\alpha\beta>}{E_{\alpha\beta}-E_{\alpha'\beta''}} + \frac{<\alpha'\beta'|V^{Ae}|\alpha\beta''><\beta''\eta+1|Ve|\beta\eta>}{E_{\alpha'\beta'}-E_{\alpha\beta''}}\right\}\delta_{\gamma'\gamma}$$

$$+ \sum_{\beta''}\left\{\frac{<\beta'\eta+1|Ve|\beta''\eta><\beta''\gamma'|V^{ie}|\beta\gamma>}{E_{\beta\gamma}-E_{\beta''\gamma'}} + \frac{<\beta'\gamma'|V^{ie}|\beta''\gamma><\beta''\eta+1|Ve|\beta\eta>}{E_{\beta'\gamma'}-E_{\beta''\gamma}}\right\}\delta_{\alpha\alpha'}$$

$$+ \sum_{\gamma''}\left\{\frac{<\gamma'\eta+1|Vi|\gamma''\eta><\alpha'\gamma''|V^{Ai}|\alpha\gamma>}{E_{\alpha\gamma}-E_{\alpha'\gamma''}} + \frac{<\alpha'\gamma'|V^{Ai}|\alpha\gamma''><\gamma''\eta+1|Vi|\gamma\eta>}{E_{\alpha'\gamma'}-E_{\alpha\gamma''}}\right\}\delta_{\beta\beta'}$$

$$+ \sum_{\alpha''}\left\{\frac{<\alpha'n+1|V_A|\alpha''\eta><\alpha''\beta'|V^{Ae}|\alpha\beta>}{E_{\alpha\beta}-E_{\alpha''\beta'}} + \frac{<\alpha'\beta'|V^{Ae}|\alpha''\beta><\alpha''\eta+1|V_A|\alpha\eta>}{E_{\alpha'\beta'}-E_{\alpha''\beta}}\right\}\delta_{\gamma\gamma'}$$

$$+ \sum_{\alpha''}\left\{\frac{<\alpha'\eta+1|V_A|\alpha''\eta><\alpha''\gamma'|V^{Ai}|\alpha\gamma>}{E_{\alpha\gamma}-E_{\alpha''\gamma'}} + \frac{<\alpha'\gamma'|V^{Ai}|\alpha''\gamma><\alpha''\eta+1|V_A|\alpha n>}{E_{\alpha'\gamma'}-E_{\alpha''\gamma}}\right\}\delta_{\beta\beta'}$$

$$+\sum_{\gamma''}\left\{\frac{<\gamma'\eta+1|V_i|\gamma''\eta><\beta'\gamma''|V^{ie}|\beta\gamma>}{E_{\beta\gamma}-E_{\beta'\gamma''}}+\frac{<\beta'\gamma'|V^{ie}|\beta\gamma''><\gamma''\eta+1|V_i|\gamma\eta>}{E_{\beta'\gamma'}-E_{\beta\gamma''}}\right\}\delta_{\alpha\alpha'}$$

(III-11)

The first sum accounts for the photon emission due to electrons moving in the field of neutral atoms. We shall refer to this as the bremsstrahlung of electrons in the field of atoms. This sum consists of two parts. The first one corresponds to the emission mechanism in which an electron interacts first with an atom through the coulomb potential and goes into an intermediate state. It then interacts with the radiation field by emitting a photon. The second part represents the emission mechanism in which an electron first emits a photon and then interacts with an atom. The second sum in eq. (III-11) is the bremsstrahlung of electrons in the field of ions and the third sum is the bremsstrahlung of ions in the field of atoms. Each of these sums contains two parts corresponding to the same emission mechanisms as described above.

The fourth (fifth and sixth) sum is the dipole radiation of atoms (atoms and ions) induced by electrons (ions and electrons). The reason we use this terminology is that the emitted radiation comes from the dipole transition of the atoms induced by the interacting electrons.

(ii) The internal states of the ions are unchanged. This implies that V_i=o because $\omega_{b'b}$=o for b'=b (see eq. (III-7)). Then the third and sixth sums in eq. (III-11) vanish and eq. (III-8) becomes

$$<n'\eta+1|V|n\eta> \;=\; <\alpha'\eta+1|V_A|\alpha\eta>\delta_{\beta\beta'}\delta_{\gamma\gamma'} \qquad \text{(III-12)}$$

under this assumption.

For structureless ions, such as hydrogen ions, V_i takes the form of eq. (III-6) for V_e. In this case, the third and sixth sums can be neglected as compared to the first two sums because the mass of hydrogen ion is much larger than the electron mass. Furthermore, eq. (III-12) is also true for this case because the free hydrogen ion, just as the free electron, can not emit or absorb any photon through direct transition.

(iii) All the cross terms after expanding the absolute square of eq. (III-8) will be neglected.

Under the above three assumptions, eq. (III-8) becomes

$$\bar{E}_\lambda(\underline{k})(f_\lambda(\underline{k})+1) = \epsilon_\lambda^{BA}(\underline{k}) + \epsilon_\lambda^{BrAe}(\underline{k}) + \epsilon_\lambda^{Brie}(\underline{k}) + \epsilon_\lambda^{DAe}(\underline{k}) + \epsilon_\lambda^{DAi}(\underline{k}) \quad \text{(III-13)}$$

where

$$\epsilon_\lambda^{BA}(\underline{k}) = \sum_{\alpha\alpha'\eta} \frac{2\pi}{\hbar} D_{\alpha\eta,\alpha\eta} |<\alpha'\eta+1|V_A|\alpha\eta>|^2 \delta(E_{\alpha'\eta+1}-E_{\alpha\eta}) \quad \text{(III-14)}$$

$$\epsilon_\lambda^{BrAe}(\underline{k}) = \sum_{\substack{\alpha\alpha'\\ \beta\beta'\eta}} \frac{2\pi}{\hbar} D_{\alpha\beta\eta,\alpha\beta\eta} \left| \sum_{\beta''} \frac{<\beta'\eta+1|V_e|\beta''\eta><\alpha'\beta''|V^{Ae}|\alpha\beta>}{E_{\alpha\beta} - E_{\alpha'\beta''}} + \sum_{\beta''} \frac{<\alpha'\beta'|V^{Ae}|\alpha\beta''><\beta''\eta+1|V_e|\beta\eta>}{E_{\alpha'\beta'}-E_{\alpha\beta''}} \right|^2 \delta(E_{\alpha'\beta'\eta+1}-E_{\alpha\beta\eta}) \quad \text{(III-15)}$$

$$\epsilon_\lambda^{Brie}(\underline{k}) = \sum_{\substack{\gamma\gamma'\\ \beta\beta'\eta}} \frac{2\pi}{\hbar} D_{\gamma\beta\eta,\gamma\beta\eta} \left| \sum_{\beta''} \frac{<\beta'\eta+1|V_e|\beta''\eta><\beta''\gamma'|V^{ie}|\beta\gamma>}{E_{\beta\gamma}-E_{\beta''\gamma'}} + \sum_{\beta''} \frac{<\beta'\gamma'|V^{ie}|\beta''\gamma><\beta''\eta+1|V_e|\beta\eta>}{E_{\beta'\gamma'}-E_{\beta''\gamma}} \right|^2 \delta(E_{\beta'\gamma'\eta+1}-E_{\beta\gamma\eta}) \quad \text{(III-16)}$$

$$\epsilon_\lambda^{DAe}(\underline{k}) = \sum_{\substack{\alpha\beta\\ \alpha'\beta'\eta}} \frac{2\pi}{\hbar} D_{\alpha\beta\eta,\alpha\beta\eta} \Bigg| \sum_{\alpha''} \frac{<\alpha'\eta+1|V_A|\alpha''\eta><\alpha''\beta'|V^{Ae}|\alpha\beta>}{E_{\alpha\beta} - E_{\alpha''\beta'}}$$

$$+ \sum_{\alpha''} \frac{<\alpha'\beta'|V^{Ae}|\alpha''\beta><\alpha''\eta+1|V_A|\alpha\eta>}{E_{\alpha'\beta'} - E_{\alpha''\beta}} \Bigg|^2 \delta(E_{\alpha'\beta'\eta+1} - E_{\alpha\beta\eta}) \qquad \text{(III-17)}$$

$$\epsilon_\lambda^{DAI}(\underline{k}) = \sum_{\substack{\alpha\alpha'\\ \gamma'\gamma\eta}} \frac{2\pi}{h} D_{\alpha\gamma\eta,\alpha\gamma\eta} \Bigg| \sum_{\alpha''} \frac{<\alpha'\eta+1|V_A|\alpha''\eta><\alpha''\gamma'|V^{Ai}|\alpha\gamma>}{E_{\alpha\gamma} - E_{\alpha''\gamma'}}$$

$$+ \sum_{\alpha''} \frac{<\alpha'\gamma'|V^{Ai}|\alpha''\gamma><\alpha''\eta+1|V_A|\alpha\eta>}{E_{\alpha'\gamma'} - E_{\alpha''\gamma}} \Bigg|^2 \delta(E_{\alpha'\gamma'\eta+1} - E_{\alpha\gamma\eta}) \qquad \text{(III-18)}$$

are the numbers of photons of momentum $\hbar\underline{k}$ and polarization λ emitted per unit time from L^3, respectively, due to the atomic bound-bound transition (ϵ_λ^{BA}), the bremsstrahlung of electrons in the field of atoms (ϵ_λ^{BrAe}) and ions (ϵ_λ^{Brie}), the atomic dipole moment transitions induced by electrons (ϵ_λ^{DAe}) and ions (ϵ_λ^{DAi}).

Since the radiation absorption due to electrons in the field of atoms will be investigated in Chapter IV, the reduction of eq. (III-15) to the form used in Chapter IV is now performed in detail.

Let the initial and final states of the electrons, the atoms and the photons in the system be

$$|\alpha\beta> = |\ldots n(\underline{K}a), n(\underline{K}'a')\ldots>|\ldots n(\underline{u}), n(\underline{u}'), n(\underline{u}'')\ldots>$$

$$|\alpha'\beta'> = |\ldots n(\underline{K}a)-1, n(\underline{K}'a')+1\ldots>|\ldots n(\underline{u})-1, n(\underline{u}')+1, n(\underline{u}'')\ldots>$$

$$|\eta> = |\ldots\eta_\lambda(\underline{k})\ldots>$$

$$|\eta+1> = |\ldots\eta_\lambda(\underline{k})+1\ldots>$$

where $n(\underline{K}a)$ is the occupation number of the atoms of the external momentum $\hbar\underline{k}$ and the internal state $|a>$. $n(\underline{u})$ is the occupation number of the electrons of momentum $\hbar\underline{u}$ and same for $\eta_\lambda(\underline{k})$. One of the intermediate states of the electrons for which the matrix elements in eq. (III-15) does not vanish is

$$|\beta''> = |\ldots n(\underline{u})-1,\ n(\underline{u}'),\ n(\underline{u}'')+1\ldots>$$

From eqs. (III-2) and (III-6), eq. (III-15) becomes

$$\epsilon_\lambda^{BrAe}(\underline{k}) = \sum_{\substack{\underline{K}a\underline{K}'a'\\ \underline{u}\underline{u}'}} \frac{4(2\pi)^4\hbar^2 e^6}{L^9 m^2\omega} \Big| \sum_{\underline{u}''} \frac{\delta_K(\underline{K}-\underline{K}'+\underline{u}-\underline{u}'')\delta_K(\underline{u}''-\underline{u}'-\underline{k})Q_{a'a}(\underline{u}-\underline{u}'')}{|\underline{u}-\underline{u}''|^2(E_{\underline{K}a}-E_{\underline{K}'a'}+E_{\underline{u}}-E_{\underline{u}''})}\underline{u}''\cdot\underline{\epsilon}_\lambda$$

$$+ \sum_{\underline{u}''} \frac{\delta_K(\underline{K}-\underline{K}'+\underline{u}''-\underline{u}')\delta_K(\underline{u}-\underline{u}''-\underline{k})Q_{a'a}(\underline{u}''-\underline{u}')}{|\underline{u}''-\underline{u}'|^2(E_{\underline{K}'a'}-E_{\underline{K}a}+E_{\underline{u}'}-E_{\underline{u}''})}\underline{u}\cdot\underline{\epsilon}_\lambda\Big|^2 \delta(E_{\underline{K}'a'}-E_{\underline{K}a}+E_{\underline{u}'}-E_{\underline{u}}+\hbar\omega)$$

$$\times N(\underline{u})N(\underline{K}a)(f_\lambda(\underline{k})+1).$$

where

$$Q_{a'a}(\underline{u}-\underline{u}') = <a'|z-\sum_{j=1}^{z} e^{i(\underline{u}-\underline{u}')\cdot\underline{\rho}_j}|a>.$$

$N(\underline{u})$, $N(\underline{K}a)$ and $f_\lambda(\underline{k})$ are the numbers of the electrons, the atoms and the photons in L^3, respectively. In obtaining the above equation, $n(\underline{u})$ and $n(\underline{K}a)$ have been neglected in comparison with unity and the statistical average over the initial particle and photon states have been performed. For non-relativistic electrons one can replace $\delta_K(\underline{u}-\underline{u}'-\underline{k})$ by $\delta_K(\underline{u}-\underline{u}')$. It means that the recoil momentum of the electrons can be neglected. Taking the sum over $\underline{u}''$ after this approximation is made, one obtains

$$\epsilon_\lambda^{BrAe}(\underline{k}) = E_\lambda^{BrAe}(\underline{k})(f_\lambda(\underline{k})+1) \qquad \text{(III-19)}$$

where

$$E_\lambda^{BrAe}(\underline{k}) = \sum_{\substack{\underline{K}a\underline{K}'a' \\ \underline{u}\,\underline{u}'}} \frac{4(2\pi)^4 e^6}{L^9 m^2 \omega^3} \frac{\delta_K(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')Q^2_{a'a}(\underline{u}-\underline{u}')}{|\underline{u}-\underline{u}'|^4} |(\underline{u}-\underline{u}')\cdot\underline{\epsilon}_\lambda|^2$$

$$\times\ \delta(E_{\underline{K}'a'}-E_{\underline{K}a}+E_{\underline{u}'}-E_{\underline{u}}+\hbar\omega)\ N(\underline{u})N(\underline{K}a) \qquad \text{(III-20)}$$

is the transition probability per unit time for emission of a photon of momentum $\hbar\underline{k}$ and polarization λ due to the bremsstrahlung of the electrons in the field of atoms.

Using the following properties

$$\sum_{\underline{K}\epsilon d^3K} \rightarrow \frac{L^3}{(2\pi)^3} d^3K$$

$$\delta_K(\underline{K}-\underline{K}'+\underline{u}-\underline{u}') \rightarrow \frac{(2\pi)^3}{L^3} \delta(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')$$

eq. (III-20) can be written as

$$E_\lambda^{BrAe}(\underline{k}) = C_\lambda^{BrAe}(\underline{k})N_A N_e \qquad \text{(III-21)}$$

where

$$C_\lambda^{BrAe}(\underline{k}) = \frac{8\pi e^6}{m^2\omega^3} \int d^3K \int d^3K' \int d^3u \int d^3u' \sum_a P_a \sum_{a'} \frac{Q^2_{a'a}(\underline{q})}{q^4} q_\lambda^2\ M_A(\underline{K})M_e(\underline{u})$$

$$\times\ \delta(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')\delta(E_{\underline{K}'a'}-E_{\underline{K}a}+E_{\underline{u}'}-E_{\underline{u}}+\hbar\omega) \qquad \text{(III-22)}$$

$$\underline{q} = u-u' \text{ and } q_\lambda = \underline{q}\cdot\underline{\epsilon}_\lambda .$$

N_A and N_e are the number densities of the atoms and electrons in the system. $P_a = N(a)|N_A$ is the ratio of the atomic density in the internal state $|a\rangle$ to the total density of the atoms in the system. It can be interpreted as the probability of finding the atoms in the state $|a>$. $M_A(\underline{K})$ and $M_e(\underline{u})$ are the distribution frequencies of the atoms in d^3K and of the electrons in d^3u. The further reduction of eq. (III-22) will be found in Chapter IV.

In the same way, the transition probabilites per unit time for photon emission due to the other mechanisms as described in eqs. (III-14), (IV-16), (III-17), and (III-18) can be written down. Letting the ion density of the system be equal to the electron density, the total transition probability per unit time for emission of a photon of momentum $\hbar\underline{k}$ and polarization λ due to all the significant mechanisms under the assumptions made is

$$E_\lambda(\underline{k}) = C_\lambda^{BA}(\underline{k})N_A + \{C_\lambda^{BrAe}(\underline{k}) + C_\lambda^{DAe}(\underline{k}) + C_\lambda^{DAi}(\underline{k})\} N_A N_e$$

$$+ C_\lambda^{Brie}(\underline{k}) N_e^2 \qquad \text{(III-23)}$$

where

$$C_\lambda^{BA}(\underline{k}) = \frac{(2\pi e)^2}{\omega} \int d^3k \sum_a P_a \sum_{a'} \omega_{a'a}^2 d_{a'a\lambda}^2(\underline{k}) M_A(\underline{K}) \delta(E_{a'} - E_a + \hbar\omega) \qquad \text{(III-24)}$$

$$C_\lambda^{Brie}(\underline{k}) = \frac{8\pi e^6}{m^2\omega^3} \int d^3\ell d^3\ell' d^3u d^3u' \sum_b P_b \sum_{b'} \frac{Q_{b'b}^2(\underline{q})}{q^4} q_\lambda^2 M_i(\underline{\ell}) M_e(\underline{u})$$

$$\times \delta(\underline{\ell} - \underline{\ell}' + \underline{u} - \underline{u}') \delta(E_{\underline{\ell}'b'} - E_{\underline{\ell}b} + E_{\underline{u}'} - E_{\underline{u}} + \hbar\omega) \qquad \text{(III-25)}$$

$$C_\lambda^{DAe}(\underline{k}) = \frac{8\pi e^6}{\hbar^2\omega} \int d^3K d^3K' d^3u d^3u' \sum_a P_a \sum_{a'} \left| \sum_{a''} \left\{ \frac{\omega_{a'a''} d_{a'a''\lambda} Q_{a''a}(\underline{q})}{\omega_{a'a''} + \omega} \right. \right.$$

$$\left. \left. - \frac{\omega_{a''a} d_{a''a\lambda} Q_{a'a''}(\underline{q})}{\omega_{a''a} + \omega} \right\} \right|^2 \frac{M_A(\underline{K}) M_e(\underline{u})}{q^4} \delta(\underline{K} - \underline{K}' + \underline{u} - \underline{u}')$$

$$\times \delta(E_{\underline{K}'a'} - E_{\underline{K}a} + E_{\underline{u}'} - E_{\underline{u}} + \hbar\omega) \qquad \text{(III-26)}$$

$$C_\lambda^{DAi}(\underline{k}) = \frac{8\pi e^6}{\hbar^2\omega} \int d^3k d^3k' d^3\ell d^3\ell' \sum_{ab} P_a P_b \sum_{a'} \frac{Q^2_{b'b}(\underline{q})}{q^4}$$

$$\times \left| \sum_{a''} \left\{ \frac{\omega_{a'a''} d_{a'a''\lambda} Q_{a''a}(\underline{q})}{\omega_{a'a''}+\omega} - \frac{\omega_{a''a} d_{a''a\lambda} Q_{a'a''}(\underline{q})}{\omega_{a''a}+\omega} \right\} \right|^2$$

$$\times M_A(\underline{K}) M_i(\underline{\ell}) \delta(\underline{K}-\underline{K}'+\underline{\ell}-\underline{\ell}') \delta(E_{\underline{K}'a'} - E_{\underline{K}a} + E_{\underline{\ell}'} - E_{\underline{\ell}} + \hbar\omega) \qquad \text{(III-27)}$$

$$d^2_{a'a\lambda} = |\underline{d}_{a'a} \cdot \underline{\epsilon}_\lambda|^2, \; Q^2_{b'b}(\underline{q}) = |\langle b'| z - \sum_{j=1}^{z-1} e^{i\underline{q}\cdot\underline{\rho}_j} |b\rangle|^2.$$

In eqs. (III-25) and (III-27), $P_b = \frac{N(b)}{N_e}$ is the probability of finding an ion in the state $|b\rangle$ and $M_i(\underline{\ell})$ describes the distribution of the ion velocities.

3. PHOTON ABSORPTION COEFFICIENT

It has been shown in section III-2 that the transition probability per unit time for emission of a photon of momentum $\hbar\underline{k}$ and polarization λ due to all the significant mechanisms $E_\lambda(\underline{k})$ is given by eq. (III-23). It is possible from $E_\lambda(\underline{k})$ to calculate the absorption coefficient for photons. This calculation is now performed.

If it is assumed that the medium is isotropic, then the absorption coefficient for unpolarized photons is

$$\alpha = \frac{1}{8\pi c} \sum_\lambda \int d\Omega_k \{A_\lambda(\underline{k}) - E_\lambda(\underline{k})\} \qquad \text{(III-28)}$$

where $A_\lambda(\underline{k})$ is the transition probability per unit time for absorption of a photon of momentum $\hbar\underline{k}$ and polarization λ.

For $M_A(\underline{K})$, $M_e(\underline{u})$ and $M_i(\underline{\ell})$ being Maxwellian distributions and for the internal states of the atoms (ions) populated as $e^{-E_a/\Theta}$ ($e^{-E_b/\Theta}$) where Θ is is the temperature of the system in energy unit, then the absorption and emission transition probability are related by the equation

$$A_\lambda(\underline{k}) = e^{\frac{\hbar\omega}{\Theta}} E_\lambda(\underline{k}). \qquad \text{(III-29)}$$

From eqs. (III-23), (III-28) and (III-29), the absorption coefficient can be written as

$$\alpha = C_o N_A + C_1 N_A N_e + C_2 N_e^2 \qquad \text{(III-30)}$$

where

$$C_o = \frac{e^{\frac{\hbar\omega}{\Theta}} - 1}{8\pi c} \sum_\lambda \int d\Omega_k C_\lambda^{BA}(\underline{k}) \qquad \text{(III-31)}$$

$$C_1 = \frac{e^{\frac{\hbar\omega}{\Theta}} - 1}{8\pi c} \sum_\lambda \int d\Omega_k \{C_\lambda^{BrAe}(\underline{k}) + C_\lambda^{DAe}(\underline{k}) + C_\lambda^{DAI}(\underline{k})\} \qquad \text{(III-32)}$$

$$C_2 = \frac{e^{\frac{\hbar\omega}{\Theta}} - 1}{8\pi c} \sum_\lambda \int d\Omega_k C_\lambda^{Brie}(\underline{k}). \qquad \text{(III-33)}$$

4. TIME-DEPENDENCE OF α

A plasma will vary with time and eventually die out if there are no external devices to maintain it. The absorption coefficient α is a function of time. The possible parameters in eq. (III-30) which may depend on time are the neutral and electron densities, the temperature of the medium and the probabilities P_a and P_b of finding respectively the atoms and the ions in the states $|a\rangle$ and $|b\rangle$. Since plasma temperatures are known to be sensitive functions of time for most cases, C_o, C_1 and C_2 are time-dependent.

In this section, we shall investigate the time variations of the quantity $y(t) = \frac{\alpha(t)}{N_{eo}^2 C_1(t)}$ instead of $\alpha(t)$, by assuming that the neutral and electron densities satisfy, respectively, the simple differential equations

$$\frac{dN_e(t)}{dt} = -\gamma_o N_e^2(t) \tag{III-34}$$

$$\frac{dN_A(t)}{dt} = \gamma_o N_e^2(t) \tag{III-35}$$

where γ_o is the recombination coefficient of the electrons with the ions. The solutions of eqs. (III-34) and (III-35) are

$$N_e(t) = \frac{N_{eo}}{1+\gamma_o N_{eo} t} \tag{III-36}$$

$$N_A(t) = N_{Ao} + \frac{\gamma_o N_{eo} t}{1+\gamma_o N_{eo} t} \tag{III-37}$$

where N_{eo} and N_{Ao} are the respectively the neutral and electron densities at the instant of the plasma formation. The substitution of eqs. (III-36) and (III-37) into eq. (III-30) gives

$$y = \frac{1}{1+x} (\lambda + \frac{x}{1+x} + \frac{\mu}{1+x}) \tag{III-38}$$

where $x = \gamma_o N_{eo} t$, $y(t) = \alpha(t)/N_{eo}^2 C_1(t)$, $\lambda = N_{Ao}|N_{eo}$ and $\mu(t) = C_2(t)/C_1(t)$ are dimensionless positive numbers. In obtaining eq. (III-38), the direct bound-bound transitions of the atomic electrons, i.e., the first term in eq. (III-30) has been neglected. The reason for neglecting this term is that it represents the atomic line absorption, and hence is negligible when the frequency of the photons is far away from the line frequencies. In eq. (III-38) λ is the ratio of the neutral to the electron density, a quantity of measuring the degree of ionization of the medium at the instant of the plasma formation. μ is the ratio of the inverse bremsstrahlung due to an electron in the field of an ion to that of an electron in the field of an atom if the contributions due to induced dipole transitions are negligible (see eq. (III-32)). In the case that $C_1(t)$ and $C_2(t)$ are sensitive to the time t, their ratio, $\mu(t)$, may be insensitive to t because the numerator and the denominator are both time dependent through the temperature in the Maxwellian distribution of particles. We shall assume that μ is constant, then a maximum of y in eq. (III-38) occurs at a value

$$x = \frac{1-\lambda-2\mu}{1+\lambda} \qquad \text{(III-39)}$$

provided $\lambda+2\mu\leq 1$ because λ, μ and x are positive numbers. The variation of $y(t)=\alpha(t)/n_{eo}^2C_1(t)$ with time is shown in Figure 1 for the plasmas with $\lambda=1/9$ and $\mu=o$, 1/9, 2/9, 3/9 and 4/9. If the dependence of plasma temperature with time is known, the variation of the absorption coefficient $\alpha(t)$ can be obtained through the calculation of $C_1(t)$.

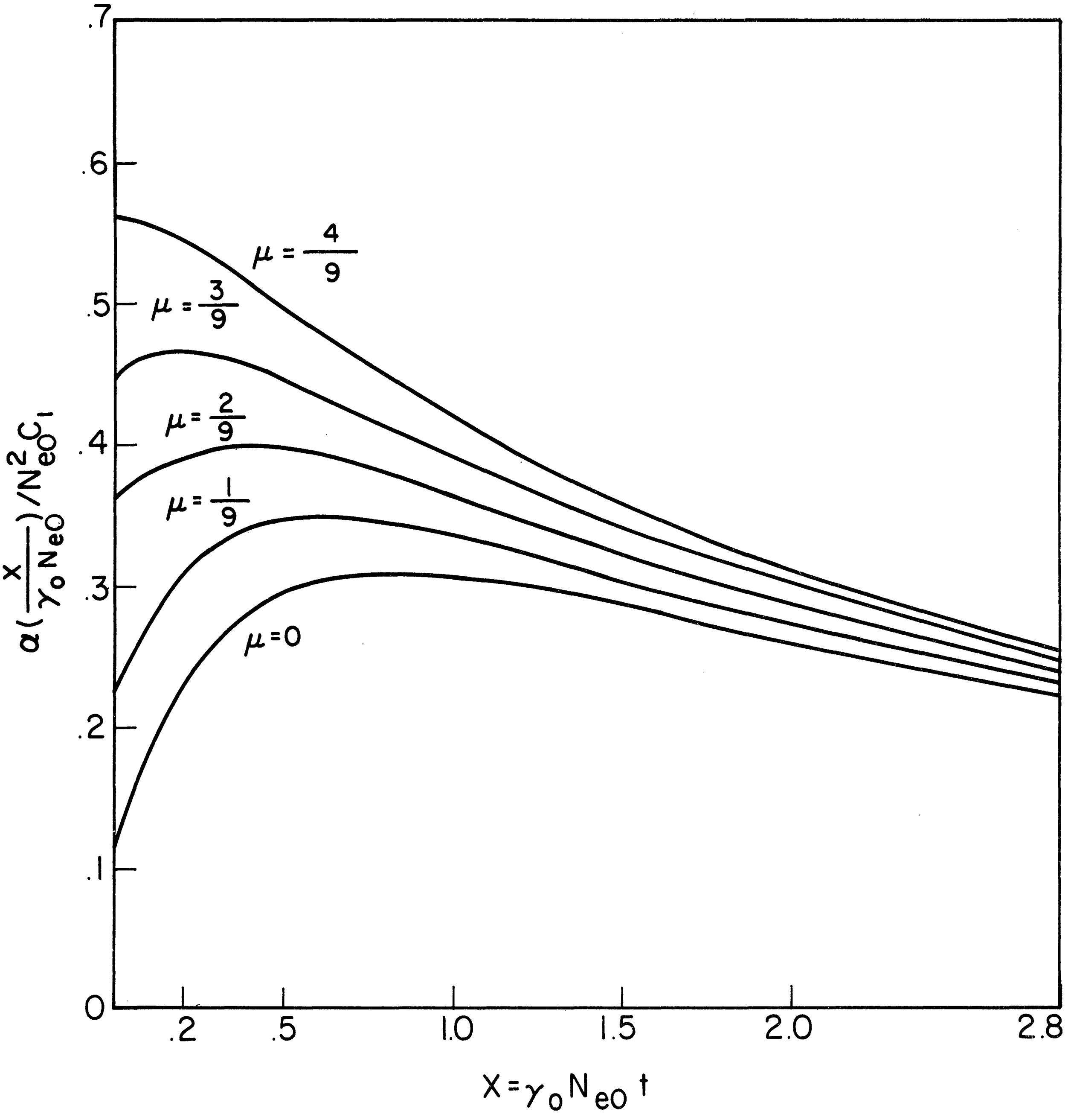

Figure 1. Variation of $\alpha(x/\gamma_o N_{eo})/N_{eo}^2 C_1$ with the time after the formation of plasma.

CHAPTER IV

RADIATION ABSORPTION IN PARTIALLY IONIZED HYDROGEN GAS DUE TO INVERSE BREMSSTRAHLUNG OF ELECTRONS IN NEUTRAL ATOMS

In 1967 Akcasu and Wald[12] investigated the radiation absorption due to the inverse bremsstrahlung of slow electrons in the field of neutral atoms. Since the temperature of the system they investigated was low ($\Theta \sim 1$ev or less), they assumed that all the atoms in the system are in the ground state, the energies of the electrons are insufficient to excite an atom from its ground state to an excited state, and the elastic scattering cross section for electron-atom collisions appearing in the absorption formula can be approximated by its value at zero electron energy. Under these assumptions they calculated the various absorption contributions due to inverse bremsstrahlung, induced dipole transition, and exchange and interference effects; and found that the last three contributions for low temperature system are negligible as compared to the first one.

For hot plasmas, such as the one[13] produced by a giant pulsed laser beam which we shall discuss later, the temperature of electrons in the plasma is about 20 eV. At such temperatures, the above assumptions made by Akcasu and Wald cannot hold. It is the aim of this chapter to consider the problem for higher electron energies. The atoms in the system are allowed initially and finally to be in any excited state as well as in the ground state. The electron energy dependence of the elastic and inelastic cross sections will be also taken into account. However, only the absorption due to the inverse bremsstrahlung of high energy electrons in the field of excited and ground atoms shall be computed. The other contributions, such as induced dipole transition, etc., which at high temperature might not be small as predicted at low temperature, will not be considered in this thesis.

1. ENERGY INTENSITY OF EMITTED RADIATION

In section III-3, we have obtained in eqs. (III-21) and (III-22) the transition probability per unit time for emission of a photon of momentum $\hbar\underline{k}$ and polarization λ due to the bremsstrahlung of the electrons in the field of atoms as

$$E_\lambda(\underline{k}) = \frac{8\pi e^6}{m^2\omega^3} \int d^3K \int d^3K' \int d^3u' \sum_a N(a) \sum_{a'} \frac{Q^2_{a'a}(q)}{q^4} q_\lambda^2 M_A(\underline{K})$$

$$\times \delta(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')\delta(E_{\underline{K}'a'}-E_{\underline{K}a}+E_{\underline{u}'}-E_{\underline{u}}+\hbar\omega) \qquad \text{(IV-1)}$$

where $N(a)=N_AP_a$ is the number of the atoms in the internal state $|a\rangle$. In eq. (IV-1) we have dropped out, for the time being, the integration $N_e\int d^3uM_e(u)$ which accounts for the effect of the Maxwellian electron distribution in order to simplify the writing of the expressions below. We shall resume this integration later in section (IV-4). The superscript BrAe in eq. (III-21) for indicating the contribution due to bremsstrahlung of the electrons in neutral atoms is also dropped out for the same reason.

For an isotropic medium, the energy intensity per unit energy emitted in all directions and in two polarizations is related to $E_\lambda(\underline{k})$ by the equation[12]

$$S(\hbar\omega) = \frac{\omega^3}{c^3(2\pi)^3} \int d\Omega_{\underline{k}} \sum_{\lambda} E_{\lambda}(\underline{k}) \qquad \text{(IV-2)}$$

where $\Omega_{\underline{k}}$ is the direction in which the photon is emitted. Recalling that $q_\lambda = \underline{q}\cdot\underline{\epsilon}_\lambda$, one has

$$\int d\Omega_{\underline{k}} \sum_{\lambda} q_\lambda^2 = \frac{8\pi}{3} q^2,$$

and eq. (IV-2) becomes

$$S(\hbar\omega) = \frac{8e^6}{3\pi m^2 c^3} \int dK^3 \int d^3K' \int d^3u' \; q^2 \sum_{aa'} N(a) \; F_{a'a}(q) M_A(\underline{K}) \delta(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')$$

$$\times \; \delta(E_{\underline{K}}-E_{\underline{K}'}+\Delta) \qquad \text{(IV-3)}$$

where

$$F_{a'a}(\underline{q}) = |\langle a' | z - \sum_{j=1}^{z} e^{i\underline{q}\cdot\underline{\rho}_j} | a \rangle|^2 / q^4$$

and

$$\Delta = E_a - E_{a'} + E_u - E_{u'} - \hbar\omega.$$

For a medium in thermal equilibrium, the atom momenta, $\hbar\underline{k}$, are distributed according to the Maxwellian distribution law, i.e.,

$$M_A(\underline{K}) d^3K = \frac{\hbar^3}{(2\pi M\Theta)^{3/2}} \; e^{-\frac{\hbar^2 K^2}{2M\Theta}} d^3K \qquad \text{(IV-4)}$$

and the integrations over d^3K and d^3K' in eq. (IV-3) can be carried out

$$S(\hbar\omega) = \frac{8e^6}{3\pi m^2 c^3} \int d^3u' \; q^2 \sum_{aa'} N(a) F_{a'a}(\underline{q}) \frac{\sqrt{M}}{\hbar q \sqrt{2\pi\Theta}} e^{-\frac{x}{4y^2}\left(\frac{\Delta}{E_{\underline{u}}} - \frac{m}{M} y^2\right)^2} \qquad \text{(IV-5)}$$

where $x = \frac{ME_{\underline{u}}}{m\Theta}$ and $y = \frac{q}{u}$. Since $d^3u' = \frac{m}{\hbar^2} u' dE_{\underline{u}} \cdot d\Omega_{\underline{u}'}$, the integration over $d\Omega_{\underline{u}'}$ can be performed and eq. (IV-5) reduces to

$$S(\hbar\omega) = \frac{16}{3}\alpha^3 \frac{1}{\hbar u^2} \int dE_{u'} \int_{q_{min}}^{q_{max}} dq q^2 \sum_{aa'} N(a) F_{a'a}(q) \left(\frac{x}{\pi}\right)^{\frac{1}{2}} e^{-\frac{x}{4y^2}\left(\frac{\Delta}{E_{\underline{u}}} - \frac{m}{M} y^2\right)^2} \quad \text{(IV-6)}$$

where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant, $q_{min} = |u-u'|$ and $q_{max} = u+u'$.

As a result of the large mass ratio $\frac{M}{m}$ of an atom to an electron, the quantity x is a large number in most cases. Therefore one can approximate the exponential factor in eq. (IV-6),

$$\left(\frac{x}{\pi}\right)^{\frac{1}{2}} \exp\left\{-\frac{x}{4y^2}\left(\frac{\Delta}{E_{\underline{u}}} - \frac{m}{M} y^2\right)^2\right\}, \text{ by } \delta\left(\frac{\Delta}{2yE_{\underline{u}}} - \frac{my}{2M}\right).$$

The last term, $my/2M$, in the argument of this delta function accounts for the recoil energy of the atom. Thus eq. (IV-6) includes the effect of finite atom mass. However, for the sake of simplicity, the atoms in the medium will be assumed to be infinitely heavy for the remainder of this chapter. Then eq. (IV-6) becomes

$$S(\hbar\omega) = \frac{16}{3}\alpha^3 \frac{\hbar}{mu} \int_0^\infty dE_{u'} \int_{q_{min}}^{q_{max}} dq\, q^3 \sum_{aa'} N(a) F_{a'a}(q) \delta(E_a - E_{a'} + E_u - E_{u'} - \hbar\omega) \quad \text{(IV-7)}$$

2. DIFFERENTIAL CROSS SECTION

In this section, we shall express the energy intensity of emitted radiation in terms of the differential cross section for electron-atom collision. During collision, the electron momentum changes from $\hbar\underline{u}$ to $\hbar\underline{u}'$ while the atom simultaneously undergoes a transition between the initial and final states $|a\rangle$ and $|a'\rangle$ for which the atom internal energies are E_a and $E_{a'}$, respectively. The differential cross section in the laboratory system of coordinates for such a process can be defined[17,18] as

$$\sigma_{aa'}(E_u,E_{u'},q)\, d\Omega_{\underline{u}'} dE_{u'}$$

$$= \frac{4}{a_o^2}\sqrt{\frac{E_{u'}}{E_{\underline{u}}}}\, F_{a'a}(q)\delta(E_a - E_{a'} + E_u - E_{u'})\, d\Omega_{\underline{u}'} dE_{u'} \tag{IV-8}$$

where $d\Omega_{\underline{u}'}$ is the element of the solid angle in the direction of $\underline{u}'$ and $a_o = \frac{\hbar^2}{me^2}$ is the first Bohr radius of hydrogen atom. The macroscopic differential cross section for the scattering process can be defined as

$$\Sigma_{aa'}(E_u,E_{u'},q) = N(a)\sigma_{aa'}(E_u,E_{u'},q) \tag{IV-9}$$

Since the various atomic transitions accompanying scattering processes remain unseparated experimentally, the macroscopic differential cross section is obtained by summing the contributions of transitions to all admissible final states of the scattering atom as

$$\Sigma_a(E_u,E_{u'},q) = \frac{4}{a_o^2}\sqrt{\frac{E_{u'}}{E_u}}\sum_{a'} N(a)F_{a'a}(q)\delta(E_a - E_{a'} + E_u - E_{u'}). \tag{IV-10}$$

Then the total macroscopic differential cross section of an electron scattered by the atoms in all possible initial states is

$$\Sigma(E_u,E_u,q) = \frac{4}{a_o^2}\sqrt{\frac{E_{u'}}{E_u}}\sum_{aa'} N(a)F_{a'a}(q)\delta(E_a - E_{a'} + E_u - E_{u'}). \tag{IV-11}$$

In terms of the differential cross section, eq. (IV-7) becomes

$$S(\hbar\omega) = \sum_{aa'} S_{aa'}(\hbar\omega) \tag{IV-12a}$$

where

$$S_{aa'}(\hbar\omega) = \frac{4}{3}\alpha^3 a_o^2 \frac{\hbar^2}{mu}\int_0^\infty dE_{u'}\sqrt{\frac{E_u}{E_{u'}+\hbar\omega}}\int_{q_{min}}^{q_{max}} dq q^3 \Sigma_{aa'}(E_u,E_{u'}+\hbar\omega,q) \tag{IV-12b}$$

or

$$S(\hbar\omega) = \frac{4}{3}\alpha^3 a_o^2 \frac{\hbar^2}{mu} \int_o^\infty dE_{u'} \sqrt{\frac{E_u}{E_{u'}+\hbar\omega}} \int_{q_{min}}^{q_{max}} dq q^3 \Sigma(E_{u'}, E_u + \hbar\omega, q). \qquad \text{(IV-12c)}$$

If all the atoms in the medium are initially and finally in the ground state as assumed by Akcasu and Wald, eqs. (IV-7) and (IV-8) become in this case

$$S(\hbar\omega) = N_A \frac{16}{3} \alpha^3 \frac{\hbar}{mu} \int_o^\infty dE_{u'} \int_{q_{min}}^{q_{max}} dq q^3 F(q) \delta(E_u - E_{u'} - \hbar\omega) \qquad \text{(IV-13)}$$

$$\sigma(q) = \frac{4}{a_o^2} F(q) \qquad \text{(IV-14)}$$

where F(q) denotes the matrix element evaluated with respect to the ground state of the atom and N_A is the number density of the atoms in the system. Equation (IV-14) is just the microscopic differential cross section of an electron elastically scattered by an atom in the ground state. In terms of the velocity, $v=\hbar u|m$, of the electron, the integral microscopic cross section can be written as

$$\sigma(v) = \frac{8\pi}{a_o^2} \int_{-1}^{1} F(q) d\mu = 8\pi\left(\frac{\hbar}{a_o m v}\right)^2 \int_o^{\frac{2mv}{\hbar}} qF(q) dq. \qquad \text{(IV-15)}$$

Combining eqs. (IV-13) and (IV-15) gives

$$S(\hbar\omega) = N_A \frac{16}{3\pi} \alpha^3 a_o^2 \left(\frac{m}{\hbar}\right)^3 \frac{1}{u} \int_o^\infty dE_{u'} \int_{v_{min}}^{v_{max}} dv v^3 \left[\sigma(v) + \frac{v}{2}\frac{d\sigma}{dv}\right]$$

$$\times \delta(E_u - E_{u'} - \hbar\omega) \qquad \text{(IV-16)}$$

where $v_{max} = \frac{v+v'}{2}$ and $v_{min} = \frac{|v-v'|}{2}$. Eq. (IV-16) indicates that the intensity of the bremsstrahlung is not determined by the value of elastic scattering cross section at the incident electron energy, as might be expected intuitively, but it depends on the variation of the cross section in the velocity region (v_{min}-v_{max}). If $\sigma(v)$ is slowly varying up to the incident energy of electrons, one can approximately evaluate the integral over dv in eq. (IV-6) for a low temperature system

$$S(\hbar\omega) = N_A \frac{4\sqrt{2}}{3\pi} \sigma(o) c \left(\frac{E_u}{mc^2}\right)^{3/2} \left(2 - \frac{\hbar\omega}{E_u}\right) \left(1 - \frac{\hbar\omega}{E_u}\right)^{\frac{1}{2}} \alpha \qquad \text{(IV-17)}$$

where $\sigma(o)$ is the cross section of the electron elastically scattered by the atom in the limit $v \to o$. Equation (IV-17) is identical to that obtained by Akcasu and Wald[12] by the partial wave method. This identity shows that the method of this chapter by using plane wave for the electron wave function will yield in the above approximation the same result as obtained by partial wave method if one uses the experimentally measured scattering cross-section of ground state atoms in both methods.

Although eq. (IV-16) is obtained by assuming that all the atoms in the medium are initially and finally in the ground state, it is also applicable to the atoms being initially and finally in the same excited state. In this case, $\sigma(v)$ in eq. (IV-16) is the cross section of an electron elastically scattered by the atoms in the excited state and N_A is replaced by N(a), the number density of the atoms in the excited state $|a\rangle$.

For inelastic scatterings of electron-atom collision, the energy intensity emitted through such processes can also be obtained from eqs. (IV-12) by knowing the differential inelastic scattering cross sections.

It is obvious that the energy intensity calculated from eqs. (IV-12) and (IV-16) will be more accurate if the experimentally determined cross sections are available. Unfortunately, the cross sections are not all experimentally measured. We shall calculate, for the sake of consistency, all the relevant cross sections in Born approximation even though some of them have been experimentally determined. In order to get various cross sections in Born approximation, one has to calculate $F_{a'a}(q)$ for various atomic states. $F_{a'a}(q)$ is also contained in eq. (IV-7), the expression for the energy intensity of emitted radiation. However, once $F_{a'a}(q)$ is calculated, one can obtain the intensity of the emitted radiation directly using eq. (IV-7) rather than first evaluating the cross section and then using eqs. (IV-12) and (IV-16).

As we shall apply the theory developed above to the hydrogen case in the next section, it is suitable here to show some of the electron-hydrogen cross sections calculated in Born approximation and partial wave method. The elastic cross sections calculated in Born approximation when the hydrogen atoms are initially and finally in the ground state $|100\rangle$ as well as in the states $|200\rangle$, $|210\rangle$, $|211\rangle$, and $|21,-1\rangle$ of the first excited energy level are given by

$$\frac{\sigma_{100}}{\pi a_o^2} = \frac{1}{3U^2}\left[7 - \frac{3U^4+9U^2+7}{(1+U^2)^3}\right]$$

$$\frac{\sigma_{200}}{\pi a_o^2} = \frac{1}{52U^2}\left[2081 - \frac{210b^6+1470b^5+4130b^4+6545b^3+6951b^2+4277b+2081}{(1+b)^7}\right]$$

$$\frac{\sigma_{210}}{\pi a_o^2} = \frac{2}{35U^2}\left[1137 - \frac{70b^6+490b^5+1470b^4+2625b^3+3087b^2+2289b+1137}{(1+b)^7}\right]$$

$$\frac{\sigma_{211}}{\pi a_o^2} = \frac{\sigma_{21-1}}{\pi a_o^2} = \frac{2}{5U^2}\left[37 - \frac{10b^4+50b^3+100b^2+95b+37}{(1+b)^5}\right]$$

where $b=4U^2$ and $U^2=u^2a_o^2$ with $\hbar^2u^2/2m$ being the incident energy of the electron. These cross sections are plotted in Figure 2 together with σ_{100}^P which is calculated by partial wave method[19,20] and agrees well with experimentally measured results[21]. σ_{100} was calculated before by Mott and Massey[17], but for the states in excited levels no elastic cross sections for electron-hydrogen collision have been calculated in either Born approximation or partial wave method. Therefore, we had to calculate σ_{200}, σ_{210} and σ_{211} using the Born approximation explicitly for the purpose of comparison with σ_{100}. For inelastic cross sections when the hydrogen atoms are initially in the ground or in an excited state, most calculations in the literature have been performed on Born approximation.[19, 22-27]

Figure 2 shows that the elastic scattering cross section for the hydrogen atom in the ground state calculated in Born approximation is less than σ_{100}^P which agrees well with the measured values. The discrepancy becomes large when the incident energy of electron decreases. Furthermore, the elastic cross section for the atom in a higher level is much larger than that for the atom in a lower level because the size of the atom is bigger. This may cause a larger radiation absorption when atoms are mostly in excited states as in the case of a hot plasma.

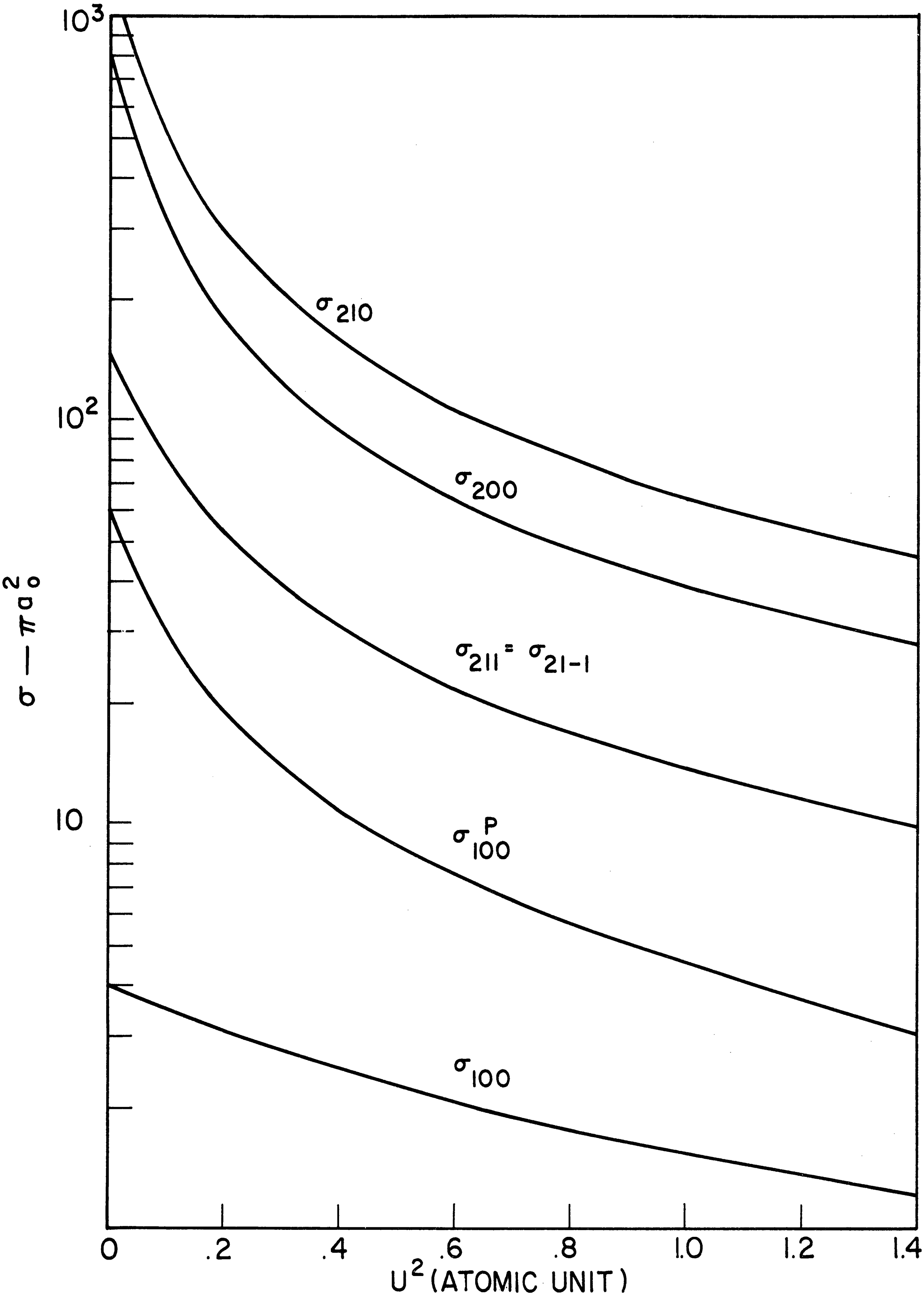

Figure 2. Elastic cross sections for hydrogen atom in the states |100>, |200>, |210>, |211>, |21-1>.

3. $\sum_{a'a} N(a)\, F_{a'a}(q)$ FOR HYDROGEN ATOM

As mentioned above, $F_{a'a}(q)$ of an atom or the scattering cross section of electron-atom collision plays an important role in the energy intensity emitted due to electrons moving in the field of atoms. Since we shall compare the radiation absorption coefficient, which is related to the emitted energy intensity (see later), to the measured values in a hydrogen plasma, we need to calculate $\sum_{a'a} N(a)\, F_{a'a}(q)$ for the hydrogen atom. Let a wave function of a hydrogen atom be labeled by $|n\ell m\rangle$ where n, ℓ, and m are, respectively, the principal, orbital angular momentum, and magnetic quantum numbers. Since the wave function of a hydrogen atom in the energy level E_n has n^2 degeneracies for a spinless orbital electron, one can write

$$\sum_{aa'} N(a) F_{a'a}(q) = \sum_{\substack{n\ell m \\ n'\ell' m'}} \frac{N(n)}{n^2 q^4} \left|\langle n'\ell' m'|1-e^{iq\cdot r}|n\ell m\rangle\right|^2 \qquad \text{(IV-18)}$$

where $N(n)$ is the number density of the hydrogen atoms in the energy E_n. In writing eq. (IV-18), we have assumed that the states of the hydrogen atoms with the same n but different possible values of ℓ and m are equally populated. Expanding the absolute square in eq. (IV-18), one can write

$$\sum_{aa'} N(a) F_{a'a}(q) = \frac{1}{q^4} \sum_{n} \frac{N(n)}{n^2} \{G(n,n,q) + \sum_{n'\neq n} G(n,n',q)\} \qquad \text{(IV-19)}$$

where

$$G(n,n,q) = n^2 - 2\,\mathrm{Re} \sum_{\ell m} \langle n\ell m|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle + \sum_{\substack{\ell m \\ \ell' m'}} \left|\langle n\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle\right|^2 \qquad \text{(IV-20)}$$

$$G(n,n',q) = \sum_{\substack{\ell m \\ \ell' m'}} |\langle n'\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle|^2. \tag{IV-21}$$

Although the elastic cross section for hydrogen atom in the ground state and some of the inelastic cross sections when the atom undergoes certain transitions have been calculated,(17, 22-27) there are no explicit expressions for $G(n,n,q)$ and $G(n,n',q)$ available in the literature except for $G(1,1,q)$, $G(1,2,q)$, $G(1,3,q)$, and $G(1,4,q)$. In order to get $G(n,n,q)$ and $G(n,n',q)$ explicitly, for other values of n and n' we shall use the method introduced by McCoyd, Milford, and Wahl(25) which we present below for completeness.

By introducing the normalized hydrogen atom wave function $|n\ell m\rangle = N_{n\ell}(r)\, Y_{\ell m}(\underline{\Omega})$ and expanding

$$e^{i\underline{q}\cdot\underline{r}} = \sum_{p=o}^{\infty} [4\pi(2p+1)]^{\frac{1}{2}} i^p j_p(qr) Y_{po}(\underline{\Omega}),$$

one can write

$$\langle n'\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle = \sum_{p=|\ell-\ell'|}^{\ell+\ell'} y_{p,\ell m,\ell' m'}\; R_{p,n\ell,n'\ell'}(q) \tag{IV-22}$$

where

$$y_{p,\ell m,\ell' m'} = i^p [4\pi(2p+1)]^{\frac{1}{2}} \int Y_{po}(\underline{\Omega}) Y_{\ell m}(\underline{\Omega}) Y^*_{\ell' m'}(\underline{\Omega}) d\Omega$$

$$= i^{p+2m'} (2p+1) \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} p & \ell & \ell' \\ o & m & -m' \end{pmatrix} \begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix} \tag{IV-23}$$

with $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ being the Wigner "3j" symbol, and

$$R_{p,n\ell,n'\ell'}(q) = \int_0^\infty N_{n\ell}(r) N^*_{n'\ell'}(r)\, j_p(qr) r^2 dr$$

$$= R_{p,n\ell,n'\ell}(\gamma) = A_{n\ell,n'\ell'} \int_0^\infty x^\beta e^{-x} j_p(\gamma x) L^{2\ell+1}_{n+\ell}(cx) L^{2\ell'+1}_{n'+\ell'}(c'x)dx \qquad \text{(IV-24)}$$

In eq. (IV-24), $j_p(\gamma x)$ are spherical Bessel functions, L^m_n are the associated Laguerre polynomials and

$$A_{n\ell,n'\ell'} = \left(\frac{2}{na_o}\right)^{\ell} \left(\frac{2}{n'a_o}\right)^{\ell'} \left(\frac{a_o nn'}{n+n'}\right)^{\ell+\ell'+3} M_{n\ell} M^*_{n'\ell'}$$

$$M_{n\ell} = -\left[\left(\frac{2}{na_o}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}\right]^{\frac{1}{2}} \qquad \text{(IV-25)}$$

$$\beta = \ell+\ell'+2, \quad c' = 2n/(n+n'), \quad c = 2n'/(n+n') \quad \gamma = qa_o nn'/(n+n')$$

From eqs. (IV-22) and (IV-23), one can perform the summations over m and m' in eq. (IV-21) by using the orthogonality property of the 3j symbol,[28]

$$\sum_{m_1=-j_1}^{+j_1} \sum_{m_2=-j_2}^{+j_2} \begin{pmatrix} j_1 j_2 j_3 \\ m_1 m_2 m_3 \end{pmatrix} \begin{pmatrix} j_1 j_2 j_3{}' \\ m_1 m_2 m_3{}' \end{pmatrix} = \frac{1}{2j_3+1}\, \delta_{j_3 j_3'}\, \delta_{m_3 m_3'}$$

then eq. (IV-21) becomes

$$G(n,n';q) = \sum_{\substack{\ell m \\ \ell' m'}} |\langle n'\ell'm'| e^{i\underline{q}\cdot\underline{r}} | n\ell m\rangle|^2 \qquad \text{(IV-26)}$$

$$= \sum_{\ell\ell' p} |R_{p,n\ell,n'\ell'}(q)|^2 (2p+1)(2\ell+1)(2\ell'+1) \begin{pmatrix} p\ell\ell' \\ 000 \end{pmatrix}^2$$

When the Laguerre functions are expressed as polynomials[29]

$$L^{2\ell+1}_{n+1}(\rho) = \sum_{s=o}^{n-\ell-1} (-1)^{S+1} \frac{\{(n+\ell)!\}^2}{(n-\ell-1-S)!(2\ell+1+S)!S!} \rho^S \qquad \text{(IV-27)}$$

the radial integral in eq. (IV-24) reduces to sums of integrals which integrate directly in terms of hypergeometric function[30]

$$\int x^{\beta'} e^{-x} j_p(\gamma x)dx = \frac{\Gamma(\frac{1}{2})\Gamma(p+\beta'+1)}{2^{p+1}\Gamma(p+\frac{3}{2})} \frac{\gamma^p}{(1+\gamma^2)^{\frac{1}{2}(p+\beta'+1)}} F\left(\frac{p+\beta'+1}{2}, \frac{p+1-\beta'}{2}, \frac{2p+3}{2}, \frac{\gamma^2}{1+\gamma^2}\right).$$

The hypergeometric function $F(a,b,c,z)$ is the analytic solution of the hypergeometric differential equation[30,31]

$$z(z-1)F'' + [(a+b+1)z-c]\,F'+abF = 0.$$

About the singularity $z=0$, it takes the form

$$F(a,b,c,z) = 1 + \frac{ab}{c} z + \frac{a(a+1)b(b+1)}{2!c(c+1)} z^2 + \ldots \qquad \text{(IV-29)}$$

where $|z|<1$. Then $F(a,b,c,z)$ will be a polynomial when a or b is a negative integer. For the terms having the odd power of x in the product of $L_{n+\ell}^{2\ell+1}(cx)$ and $L_{n'+\ell'}^{2\ell'+1}(c'x)$, one can prove that $b = \frac{p+1-\beta'}{2}$ is a negative integer and $b\leq -1$. Therefore the radial integral of eq. (IV-28) will be a polynomial for these terms. If a or b is not a negative integer, $F(a,b,c,z)$ should be expressed about the singularity at $z=1$ instead of $z=0$

$$F(a,b,c,z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} F(a,b,1+a+b-c,1-z)$$

$$+ \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} (1-z)^{c-a-b} F(c-a,c-b,1+c-a-b,1-z) \qquad \text{(IV-30)}$$

then $F(a,b,c,z)$ is a polynomial in $(1-z)$ because c-a is a negative integer or zero for the terms having the even power of x in the product of $L_{n+\ell}^{2\ell+1}(cx)$

and $L^{2\ell'+1}_{n'+\ell'}$ (c'x). The first term in eq. (IV-30) vanishes because $\Gamma(c-a)\to\pm\infty$ when c-a approaches a negative integer or zero.

With the tabulated values of the "3j" symbols and the above described calculation of the radial integral, one can, in principle, find G(n,n,q) and G(n,n',q) for any values of n and n'. It is obvious that the calculations for large values of n and n' are tedious. We shall calculate G(n,n,q) and G(n,n',q) only for n,n'=1,2,3 below.

From eqs. (IV-20), (IV-22), (IV-23), and (IV-26) and from the tabulated the "3j" symbols,[32] one can obtain (see Appendix D)

$$G(1,1,q) = \{1-R_{0,10,10,}(q)\}^2 \qquad \text{(IV-31a)}$$

$$G(1,2,q) = R^2_{0,10,20}(q) + 3R^2_{1,10,21}(q) \qquad \text{(IV-31b)}$$

$$G(1,3,q) = R^2_{0,10,30}(q) + 3R^2_{1,10,31}(q) + 5R^2_{2,10,32}(q) \qquad \text{(IV-31c)}$$

$$G(2,2,q) = 4-2R_{0,20,20}(q) + R^2_{0,20,20,}(q)-6R_{0,21,21,}(q)$$
$$+ 3R^2_{0,21,21}(q) + 6R^2_{2,21,21}(q) + 6R^2_{1,20,21}(q) \qquad \text{(IV-31d)}$$

$$G(2,3,q) = R^2_{0,20,30}(q) + 3R^2_{1,20,31}(q) + 5R^2_{2,20,32}(q) + 3R^2_{1,21,30}(q)$$
$$+ 3R^2_{0,21,31}(q) + 6R^2_{2,21,31}(q) + 6R^2_{1,21,32}(q) + 9R^2_{3,21,32}(q) \qquad \text{(IV-31e)}$$

$$G(3,3,q) = 9-2R_{0,30,30}(a) + R^2_{0,30,30}(q) -6R_{0,31,31}(q) + 3R^2_{0,31,31}(q)$$
$$+ 6R^2_{2,31,31}(q) -10R_{0,32,32}(q) + 5R^2_{0,32,32}(q) + \frac{50}{7} R^2_{2,32,32}(q)$$

$$+ \frac{90}{7} R^2_{4,32,32}(q) + 6R^2_{1,30,31}(q) + 10R^2_{2,30,32}(q) + 12R^2_{1,31,32}(q)$$

$$+ 18R^2_{3,31,32}(q). \qquad \text{(IV-31f)}$$

where $R_{p,n\ell,n'\ell'}(q)$ are determined by eqs. (IV-24) thru (IV-30). From straightforward but tedious manipulations, one obtains $R_{p,n\ell,n'\ell'}(q)$ for n and n'=1,2,3 with the following results:

$$R_{0,10,10}(q) = \frac{1}{\left(1 + \frac{q^2a_o^2}{4}\right)^2}$$

$$R_{0,10,20}(q) = 2^{\frac{17}{2}} \frac{q^2a_o^2}{(9+4q^2a_o^2)^3}$$

$$R_{1,10,21}(q) = 2^{\frac{15}{2}} 3^{\frac{1}{2}} \frac{qa_o}{(9+4q^2a_o^2)^3}$$

$$R_{0,10,30}(q) = \frac{3^{\frac{3}{2}} \xi^2(4+3\xi^2)}{(4+\xi^2)^4}$$

$$R_{1,10,31}(q) = 3^{\frac{3}{2}} 2^{\frac{1}{2}} \frac{\xi(4+3\xi^2)}{(4+\xi^2)^4}$$

$$R_{2,10,32}(q) = \frac{2^{\frac{5}{2}} 3^{\frac{3}{2}}}{5^{1/2}} \frac{\xi^2}{(4+\xi^2)^4}$$

$$R_{0,20,20}(q) = \frac{2q^4a_o^4-3q^2a_o^2+1}{(1+q^2a_o^2)^4}$$

$$R_{1,20,21}(q) = 3^{\frac{1}{2}} \frac{qa_o(q^2a_o^2-1)}{(1+q^2a_o^2)^4} \qquad \text{(IV-32)}$$

$$R_{0,21,21}(q) = -\frac{q^2a_o^2-1}{(1+q^2a_o^2)^4}$$

$$R_{2,21,21}(q) = \frac{2q^2a_o^2}{(1+q^2a_o^2)^4}$$

$$R_{0,20,30}(q) = \frac{2^{\frac{13}{2}}3^{\frac{3}{2}}}{5^6}\ \gamma^2\ \frac{75\gamma^4-194\gamma^2+115}{(1+\gamma^2)^5}$$

$$R_{1,20,31}(q) = \frac{2^9 3^{\frac{3}{2}}}{5^6}\ \frac{\gamma(15\gamma^4-28\gamma^2+5)}{(1+\gamma^2)^5}$$

$$R_{2,20,32}(q) = \frac{2^{13}3^{\frac{3}{2}}}{5^{\frac{13}{2}}}\ \frac{\gamma^2(\gamma^2-2)}{(1+\gamma^2)^5}$$

$$R_{1,21,30}(q) = \frac{2^{\frac{13}{2}}3^2}{5^6}\ \frac{\gamma(45\gamma^4-78\gamma^2+5)}{(1+\gamma^2)^5}$$

$$R_{0,21,31}(q) = \frac{2^{10}3^2}{5^6}\ \frac{\gamma^2(3\gamma^2-5)}{(1+\gamma^2)^5}$$

$$R_{2,21,31}(q) = \frac{2^{11}3^2}{5^6}\ \frac{\gamma^2(3\gamma^2-1)}{(1+\gamma^2)^5}$$

$$R_{1,21,32}(q) = \frac{2^{10}3^2}{5^{\frac{13}{2}}}\ \frac{\gamma(3\gamma^2-5)}{(1+\gamma^2)^5}$$

$$R_{3,21,32}(q) = \frac{2^{13}3^2}{5^{13/2}}\ \frac{\gamma^3}{(1+\gamma^2)^5} \qquad \text{(IV-32)}$$

$$R_{0,30,30}(q) = \frac{9\xi^8-48\xi^6+72\xi^4-28\xi^2+3}{3(1+\xi^2)^6}$$

$$R_{1,30,31}(q) = \frac{2^{\frac{1}{2}}}{3}\,\frac{\xi(9\xi^6-36\xi^4+29\xi^2-6)}{(1+\xi^2)^6}$$

$$R_{2,30,32}(q) = \frac{2^{\frac{5}{2}}}{3\sqrt{5}}\,\frac{\xi^2(3\xi^4-12\xi^2+5)}{(1+\xi^2)^6}$$

$$R_{0,31,31}(q) = -\,\frac{12\xi^6-43\xi^4+22\xi^2-3}{3(1+\xi^2)^6}$$

$$R_{2,31,31}(q) = \frac{2^3}{3}\,\frac{\xi^2(3\xi^4-5\xi^2+2)}{(1+\xi^2)^6}$$

$$R_{1,31,32}(q) = -\,\frac{5^{\frac{1}{2}}}{3}\,\frac{\xi(3\xi^4-10\xi^2+3)}{(1+\xi^2)^6}$$

$$R_{3,31,32}(q) = \frac{2^3 5^{\frac{1}{2}}}{3}\,\frac{\xi^3(\xi^2-1)}{(1+\xi^2)^6}$$

$$R_{0,32,32}(q) = \frac{3\xi^4-10\xi^2+3}{3(1+\xi^2)^6}$$

$$R_{2,32,32}(q) = -\,\frac{2^3}{3\cdot 5}\,\frac{\xi^2(3\xi^2-7)}{(1+\xi^2)^6} \qquad \text{(IV-32)}$$

$$R_{4,32,32}(q) = \frac{2^4}{3} \frac{\xi^4}{(1+\xi^2)^6}$$

where $\xi = \frac{3}{2}qa_o$ and $\gamma = \frac{6}{5}qa_o$. The substitution of eqs. (IV-32) into eqs. (IV-31) gives, by a straightforward manipulation,

$$G(1,1,q) = \{1- \frac{1}{\left(\frac{4+q^2a_o^2}{4}\right)^2}\}^2 \tag{IV-33}$$

$$G(1,2,q) = \frac{2^{15}q^2a_o^2}{(9+4q^2a_o^2)^5} \tag{IV-34}$$

$$G(1,3,q) = \frac{81x(3x+2)}{(4+x)^6} , \quad x = \frac{9}{4} q^2a_o^2 \tag{IV-35}$$

$$G(2,2,q) = 2x\{\frac{2}{1+x} + \frac{2}{(1+x)^2} + \frac{10}{(1+x)^4} - \frac{5}{(1+x)^6}\} , \quad x=q^2a_o^2 \tag{IV-36}$$

$$G(2,3,q) = \frac{2^{13}3^4}{5^{11}} x\{\frac{375}{(1+x)^5} - \frac{1160}{(1+x)^6} + \frac{1728}{(1+x)^7}\} \quad x = \frac{36}{25}q^2a_o^2 \tag{IV-37}$$

$$G(3,3,q) = x\{\frac{9}{1+x} + \frac{9}{(1+x)^2} + \frac{3}{(1+x)^3} + \frac{83}{(1+x)^4} - \frac{256}{(1+x)^5} + \frac{260}{(1+x)^6} + \frac{140}{(1+x)^7} - \frac{140}{(1+x)^8}\} , \quad x = \frac{9}{4}q^2a_o^2 \tag{IV-38}$$

Equations (IV-34) and (IV-35) are identical with the results obtained by R. McCarroll[22] using a method introduced by Mott and Massey.[17]

4. RADIATION ABSORPTION IN PARTIALLY IONIZED HYDROGEN PLASMA

With expressions of $G(n,n';q)$ obtained in the last section, the energy intensity emitted for the atom undergoing the transition from the level E_n to $E_{n'}$ and for Maxwellian electron distribution $2\pi(\pi\Theta)^{-\frac{3}{2}} N_e E_u^{\frac{1}{2}} e^{-\frac{E_u}{\Theta}}$ can be obtained from eq. (IV-7)

$$S_{nn'}(\hbar\omega) = \frac{32}{3\sqrt{2}} \frac{\hbar^2 \pi \alpha^3}{(\pi\Theta m)^{3/2}} N_e \int_0^\infty dE_u e^{-\frac{E_u}{\Theta}} \int_0^\infty dE_{u'} \int_{q_{min}}^{q_{max}} \frac{dq}{q} \frac{N(n)}{n^2} G(n,n';q)$$

$$\times \delta(E_n - E_{n'} + E_u - E_{u'} - \hbar\omega). \tag{IV-39}$$

Since the radiation emission coefficient per unit length for an isotropic medium and unpolarized radiation is given by

$$E(\hbar\omega) = \frac{1}{8\pi c} \int d\Omega_k \sum_\lambda E_\lambda(\underline{k}), \tag{IV-40}$$

one obtains from eq. (IV-2)

$$E_{nn'}(\hbar\omega) = \frac{\pi^2 c^2}{\omega^3} S_{nn'}(\hbar\omega)$$

$$= \frac{32}{3\sqrt{2}} \frac{\hbar^2 \pi^3 c^2 \alpha^3}{(\pi\Theta m)^{3/2} \omega^3} N_e \int_0^\infty dE_u e^{-\frac{E_u}{\Theta}} \int_0^\infty dE_{u'} \int_{q_{min}}^{q_{max}} \frac{dq}{q} \frac{N(n)}{n^2} G(n,n';q)$$

$$\times \delta(E_n - E_{n'} + E_u - E_{u'} - \hbar\omega) \tag{IV-41}$$

for the particular emission process $E_u + E_n \rightarrow E_{u'} + E_{n'} + \hbar\omega$. Its inverse process, i.e., $E_{u'} + E_{n'} + \hbar\omega \rightarrow E_u + E_n$, is the one for radiation absorption, and the absorption per unit length can be obtained by interchanging $(\underline{u},\underline{u}')$ and (n,n')

$$A_{n'n}(\hbar\omega) = \frac{32}{3\sqrt{2}} \frac{\hbar^2\pi^3c^2\alpha^3}{(\pi\Theta m)^{3/2}\omega^3} N_e \int_0^\infty dE_{u'} e^{-\frac{E_{u'}}{\Theta}} \int_0^\infty dE_u \int_{q_{min}}^{q_{max}} \frac{dq}{q} \frac{N(n')}{n'^2} G(n',n,q)$$

$$\times \delta(E_{n'}-E_n+ E_{u'}-E_u+\hbar\omega). \qquad \text{(IV-42)}$$

Then the absorption coefficient, i.e., the net absorption per unit length, is (by noting that $G(n,n',q)=G(n',n,q)$)

$$\alpha_{nn'}(\hbar\omega) = A_{n'n}(\hbar\omega) - E_{nn'}(\hbar\omega)$$

$$= \frac{32}{3\sqrt{2}} \frac{\hbar^2\pi^3c^2\alpha^3}{(\pi\Theta m)^{3/2}\omega^3} N_e \int_0^\infty dE_u \int_0^\infty dE_{u'} \int_{q_{min}}^{q_{max}} \frac{dq}{q} G(n,n'q)$$

$$\times \frac{N(n)}{n^2} e^{-\frac{E_u}{\Theta}} \{\frac{n^2}{n'^2}\frac{N(n')}{N(n)} e^{-\frac{E_{u'}-E_u}{\Theta}} -1\} \delta(E_n-E_{n'}+E_u-E_{u'}-\hbar\omega). \qquad \text{(IV-43)}$$

For thermal equilibrium, the number densities of hydrogen atoms are populated as

$$\frac{N(n')}{N(n)} = \frac{n'^2}{n^2} e^{-\frac{E_{n'}-E_n}{\Theta}} \qquad \text{(IV-44)}$$

then

$$\alpha_{nn'}(\hbar\omega) = N_e C_o (e^{\frac{\hbar\omega}{\Theta}}-1) \int_0^\infty dE_u e^{-\frac{E_u}{\Theta}} \int_0^\infty dE_{u'} \int_{q_{max}}^{q_{max}} \frac{dq}{q} \frac{N(n)}{n^2} G(n,n',q)$$

$$\times \delta(E_n-E_{n'}+E_u-E_{u'}-\hbar\omega) \qquad \text{(IV-45)}$$

where

$$C_o = \frac{32}{3\sqrt{2}} \frac{\hbar^2\pi^3c^2\alpha^3}{(\pi\Theta m)^{3/2}\omega^3} . \qquad \text{(IV-46)}$$

Substituting eqs. (IV-33) through (IV-38) into eq. (IV-45), one finally obtains $\sigma_{nn'}(h\omega)$ as

$$\alpha_{nn}(\hbar\omega) = C_o(e^{\frac{\hbar\omega}{\Theta}}-1)\hbar\omega\; g_{nn}(\hbar\omega,\Theta)\; N(n)N_e \tag{IV-47}$$

for n = n', and as

$$\alpha_{nn'}(\hbar\omega) = C_o(e^{\frac{\hbar\omega}{\Theta}}-1)\hbar\omega\; g^{\pm}_{nn'}(\hbar\omega,\Theta)\; N(n)N_e \tag{IV-48}$$

for $n \neq n'$. Here the upper sign of $g_{nn'}$ is to be taken when $n<n'$, and the lower sign when $n>n'$. The definitions of g_{nn}, $g^{+}_{nn'}$ and $g^{-}_{nn'}$ are given below with the convention that $g^{-}_{nn'} = g^{-}_{n'n}\, N(n')/N(n)$.

$$g_{11}(\hbar\omega,\Theta) = \frac{1}{2}\int_1^\infty dx\{\ell n\,\frac{1+d_+}{1+d_-} + \frac{6d_-^2+9d_-+1}{6(1+d_-)^3} - \frac{6d_+^2+9d_++1}{6(1+d_+)^3}\}e^{-\frac{\hbar\omega}{\Theta}x} \tag{IV-47a}$$

$$g_{22}(\hbar\omega,\Theta) = \frac{1}{4}\int_1^\infty dx\{2\ell n\,\frac{1+b_+}{1+b_-} + \frac{6b_-^4+24b_-^3+46b_-^2+44b_-+13}{3(1+b_-)^5}$$

$$- \frac{6b_+^4+24b_+^3+46b_+^2+44b_++13}{3(1+b_+)^5}\}e^{-\frac{\hbar\omega}{\Theta}x} \tag{IV-47b}$$

$$g_{33}(\hbar\omega,\Theta) = \frac{1}{18}\int_1^\infty dx\;\{9\ell n\,\frac{1+S_+}{1+S_-} + \frac{54S_-^6+333S_-^5+1021S_-^4+1450S_-^3+1056S_-^2+645S_-+177}{6(1+S_-)^7}$$

$$- \frac{54S_+^6+333S_+^5+1021S_+^4+1450S_+^3+1056S_+^2+645S_++177}{6(1+S_+)^7}\}e^{-\frac{\hbar\omega}{\Theta}x} \tag{IV-47c}$$

$$g^{\pm}_{12}(\hbar\omega,\Theta) = 2^{10} f^{\pm}_{12}\epsilon^{\pm}_{12}\int_1^\infty dx\{\frac{1}{(9+4\epsilon^{\pm}_{12}b_-)^4} - \frac{1}{(9+4\epsilon^{\pm}_{12}b_+)^4}\}e^{-\frac{\epsilon^{\pm}_{12}\hbar\omega}{\Theta}x} \tag{IV-48a}$$

$$g^{\pm}_{13}(\hbar\omega,\Theta) = \frac{81}{8} f^{\pm}_{13}\epsilon^{\pm}_{13} \int_1^\infty dx \left\{\frac{3\epsilon^{\pm}_{13} S_-+4}{(\epsilon^{\pm}_{13}S_-+4)^5} - \frac{3\epsilon^{\pm}_{13}S_++4}{(\epsilon^{\pm}_{13}S_++4)^5}\right\} e^{-\frac{\epsilon^{\pm}_{13}\hbar\omega}{\Theta}x} \quad \text{(IV-48b)}$$

$$g^{\pm}_{23}(\hbar\omega,\Theta) = \frac{2^8 3^4}{5^{11}} f^{\pm}_{23}\epsilon^{\pm}_{23} \int_1^\infty dx \left\{\frac{375(\epsilon^{\pm}_{23}\beta_-)^2-178(\epsilon^{\pm}_{23}\beta_-)+599}{(1+\epsilon^{\pm}_{23}\beta_-)^6}\right.$$

$$\left. - \frac{375(\epsilon^{\pm}_{23}\beta_+)^2-178(\epsilon^{\pm}_{23}\beta_+)+599}{(1+\epsilon^{\pm}_{23}\beta_+)^6}\right\} e^{-\frac{\epsilon^{\pm}_{23}\hbar\omega}{\Theta}x} \quad \text{(IV-48c)}$$

$$b_{\pm} = \frac{2ma_o^2\hbar\omega}{\hbar^2}(\sqrt{x} \pm \sqrt{x-1})^2,\ d_{\pm} = \frac{1}{4} b_{\pm},\ S_{\pm} = \frac{9}{4} b_{\pm} \quad \text{(IV-47d)}$$

$$\beta_{\pm} = \frac{36}{25} b_{\pm},\ \epsilon^{\pm}_{nn'} = \left|\frac{E_{n'}-E_n}{\hbar\omega} \pm 1\right|,\ f^{+}_{nn'} = 1$$

$$f^{-}_{nn'} = e^{-\frac{\hbar\omega}{\Theta}} \quad \text{for } \hbar\omega < E_{n'}-E_n$$

$$= e^{-\frac{E_{n'}-E_n}{\Theta}} \quad \text{for } \hbar\omega > E_{n'}-E_n \quad \text{(IV-48d)}$$

For $\hbar\omega=E_{n'}-E_n$, $g^{-}_{nn'}(\hbar\omega,\Theta)$ will be evaluated by

$$g^{-}_{12}(\hbar\omega,\Theta) = (\tfrac{2}{3})^9\, e^{-\frac{E_2-E_1}{\Theta}}\, \frac{\Theta}{\hbar\omega} \{6-2c_1+c_1^2-c_1^3+c_1^4 e^{c_1} E_1(c)\} \quad \text{(IV-48f)}$$

$$g^{-}_{13}(\hbar\omega,\Theta) = \frac{3^3}{2^{13}}\, e^{-\frac{E_3-E_1}{\Theta}}\, \frac{\Theta}{\hbar\omega}\{12-6c_2+4c_2^2\ 5c_2^3-c_2^4+c_2^4 e^{c_2}(6+c_2)E_1(c_2)\} \quad \text{(IV-48g)}$$

$$g^{-}_{23}(\hbar\omega,\Theta) = \frac{2^8 3^4}{5^{11}} e^{-\frac{E_3-E_2}{\Theta}} \frac{\Theta}{\hbar\omega} \{599 - \frac{671}{5} c_3 + \frac{1283}{30} c_3^2 - \frac{1291}{30} c_3^3$$

$$- \frac{436}{15} c_3^4 - \frac{48}{5} c_3^5 + c_3^4 e^{c_3}(\frac{125}{5} + \frac{116}{3} c_3 + \frac{48}{5} c_3^2)E_1(c_3)\} \qquad \text{(IV-48h)}$$

where

$$c_1 = \frac{9\hbar^2}{32ma_o^2\Theta}, \quad c_2 = \frac{2\hbar^2}{9ma_o^2\Theta}, \quad c_3 = \frac{25\hbar^2}{288ma_o^2\Theta}, \quad E_1(x) = \int_1^\infty \frac{dy}{y} e^{-xy} \qquad \text{(IV-48k)}$$

The above expressions of $g^{+}_{nn'}$ and $g^{-}_{nn'}$ are obtained from eq. (IV-45) considering the cases n<n' and n>n' separately. The property that G(n,n',q)=G(n',n,q) and the population law for thermal equilibrium, i.e., eq. (IV-44), have been used in obtaining eq. (IV-48). The values of $E_1(x)$ are available in tabulated form.[33] $g_{nn'}(\hbar\omega,\Theta)$ and $g^{\pm}_{nn'}(\hbar\omega,\Theta)$ are dimensionless numbers which we have calculated numerically. Figures 3 through 11 show the results of the computations for $g_{nn}(\hbar\omega,\Theta)$ and $g^{\pm}_{nn'}(\hbar\omega,\Theta)$ as functions of $\hbar\omega$ and T. $g^{\pm}_{nn'}$ is about 10 times less at high temperature and much less at low temperature than g_{nn}.

5. VALUES OF $g_{nn}(\hbar\omega,\Theta)$ FOR $n>3$.

As seen in sections IV-3 and IV-4, the value of $g_{nn}(\hbar\omega,\Theta)$ is obtained through the calculation of G(n,n,q) which is tedious for $n>3$. Here we shall use interpolation, instead of the direction calculation through the method in section IV-3, to get the values of $g_{nn}(\hbar\omega,\Theta)$ for $n>3$ by knowing that the absorption coefficient due to inverse bremsstrahlung of an electron in the field of a neutral atom becomes the absorption coefficient due to inverse bremsstrahlung of an electron in the field of an ion when n goes to infinity, i.e.,

$$\lim_{n\to\infty} \frac{\alpha_{nn}(\hbar\omega,\Theta)}{N(n)N_e} = \frac{\alpha^{BI}(\hbar\omega,\Theta)}{N_I N_e} \qquad \text{(IV-49)}$$

where N_I is the number density of ions and $\alpha^{BI}(\hbar\omega,\Theta)$ is the absorption coefficient due to inverse bremsstrahlung of electrons in the field of ions. $\alpha^{BI}(\hbar\omega,\Theta)$ has been given(13) for hydrogen atom as

$$\alpha^{BI}(\hbar\omega,\Theta) = \frac{8}{3(3\pi)^{1/2}} \frac{c^2}{\hbar} (\alpha a_o)^3 \frac{E^{3/2}}{\Theta^{1/2}\nu^3} g_{ff} N_I N_e \qquad \text{(IV-50)}$$

where ν is the frequency of the radiation, E is the ionization potential of a hydrogen atom and g_{ff} is the free-free Gaunt factor(34,35) depending on temperature and the absorbed radiation frequency. With the value of g_{ff}, one can find the upper bound of g_{nn} when $n\to\infty$ through eqs. (IV-47), (IV-49), and (IV-50). Since we shall compare our calculated absorption coefficients with the measured results which were achieved for the ruby laser frequency under six different temperatures, the upper bounds are obtained for these conditions and plotted as $\frac{1}{n^2}$ in Figure 12 together with g_{11}, g_{22}, and g_{33} obtained from Figures 3 through 5. Then the values of g_{nn} for $n>3$ can be obtained by interpolation on the smooth curve which is connected through the values of g_{11}, g_{22}, g_{33} and the upperbound.

Since $g^{\pm}_{nn'}$ is about ten times less than g_{nn} when n=1 and is getting much less than g_{nn} when n and n' both increase, the contributions to the

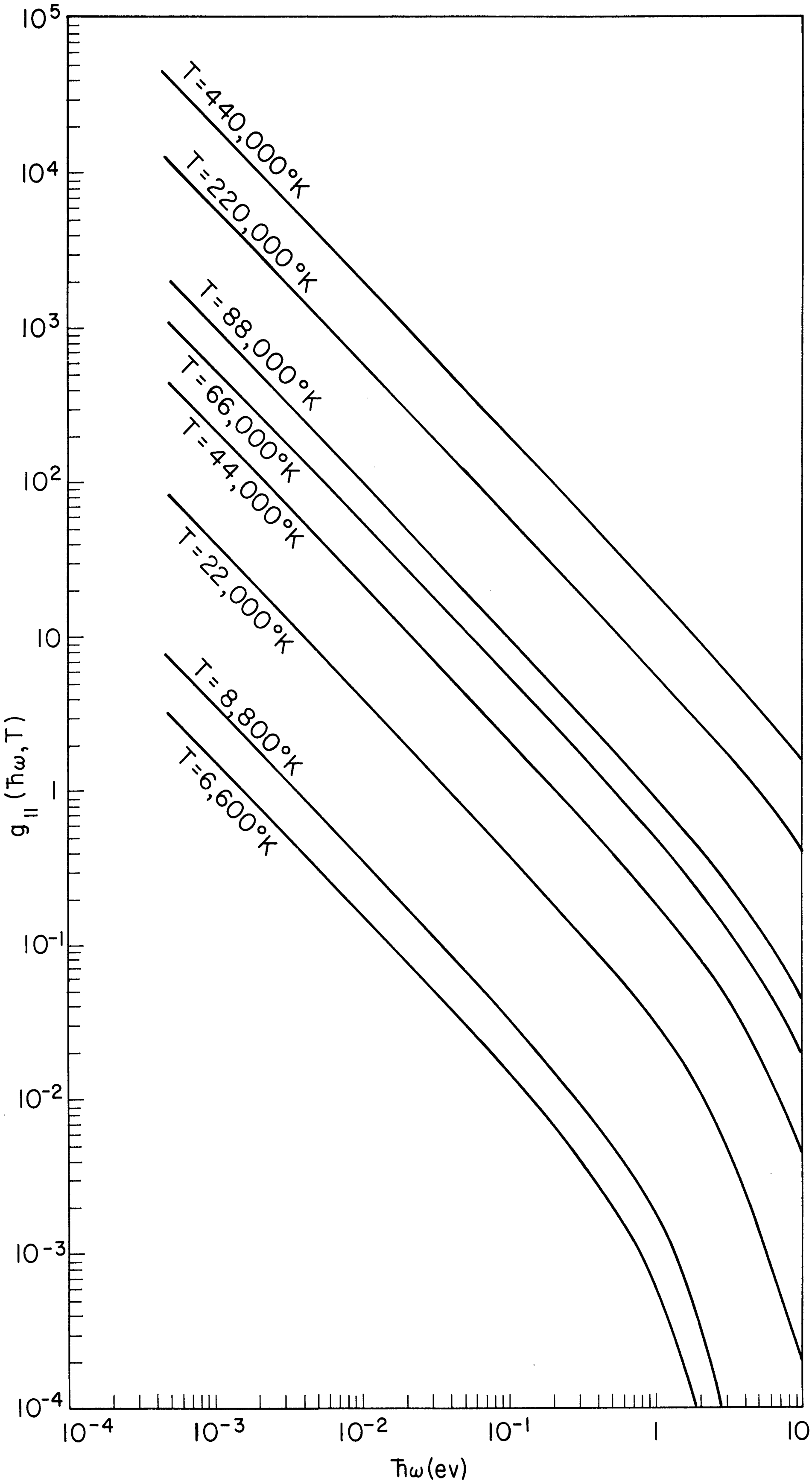

Figure 3. $g_{11}(\hbar\omega, T)$.

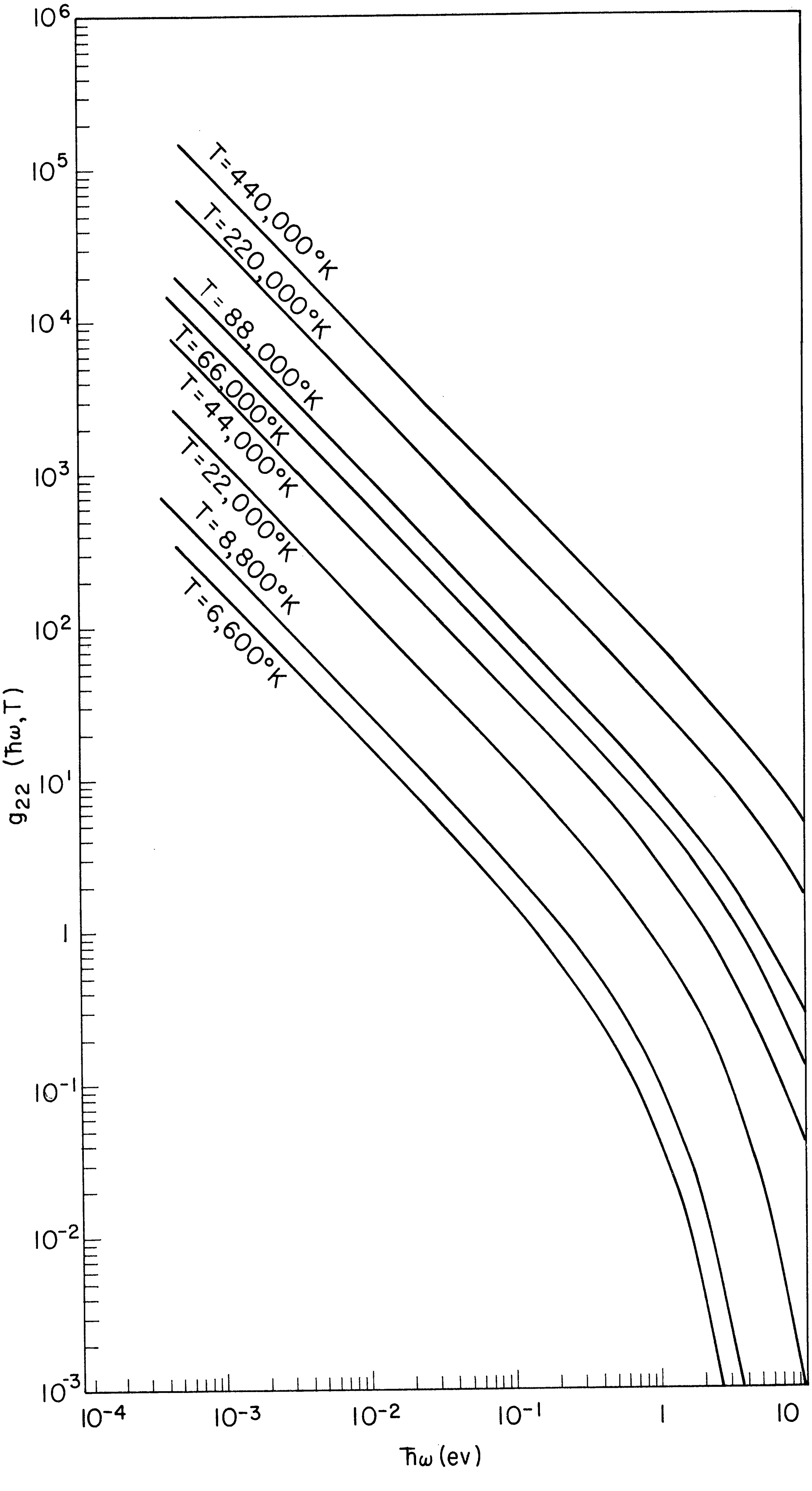

Figure 4. $g_{22}(\hbar\omega, T)$.

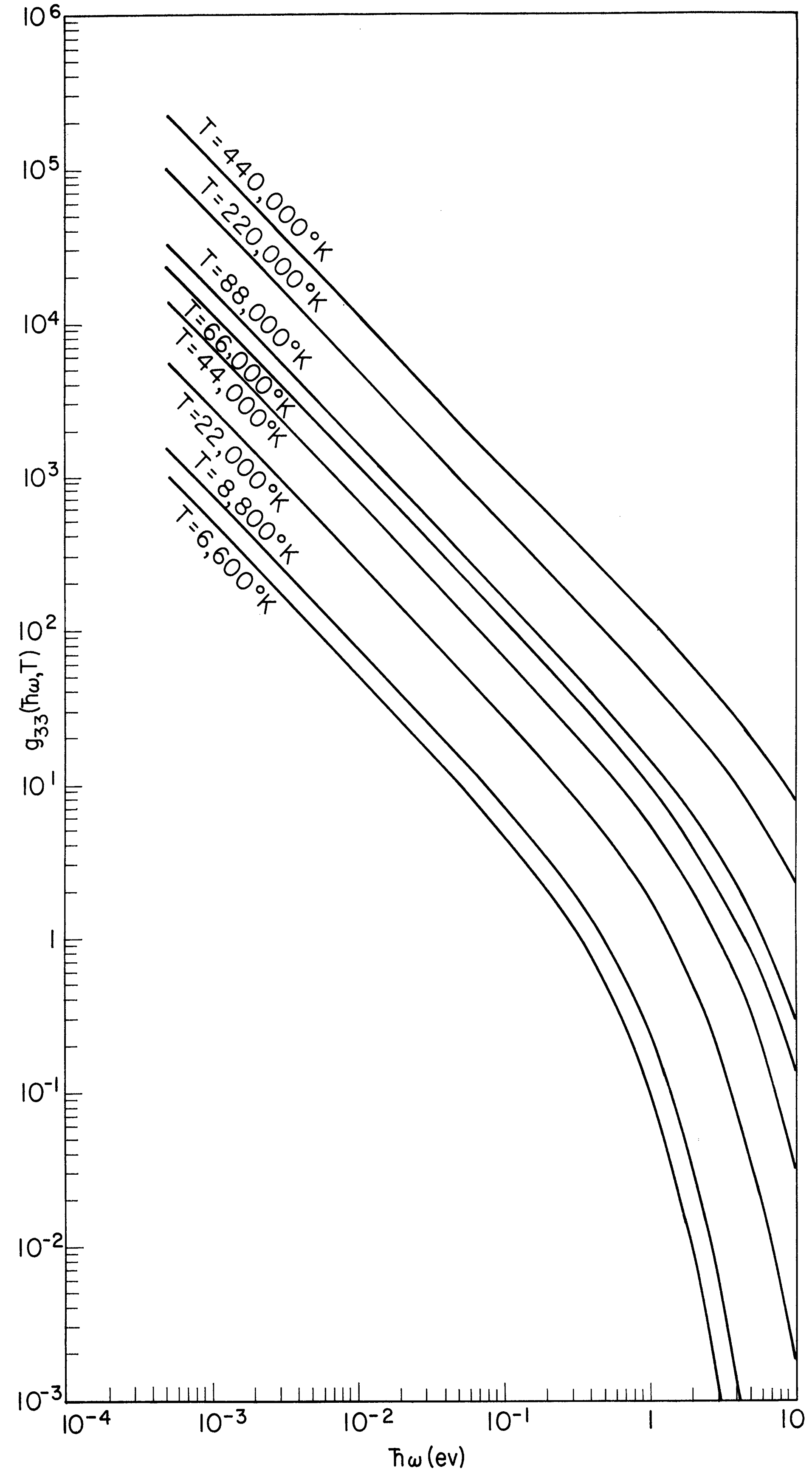

Figure 5. $g_{33}(\hbar\omega, T)$.

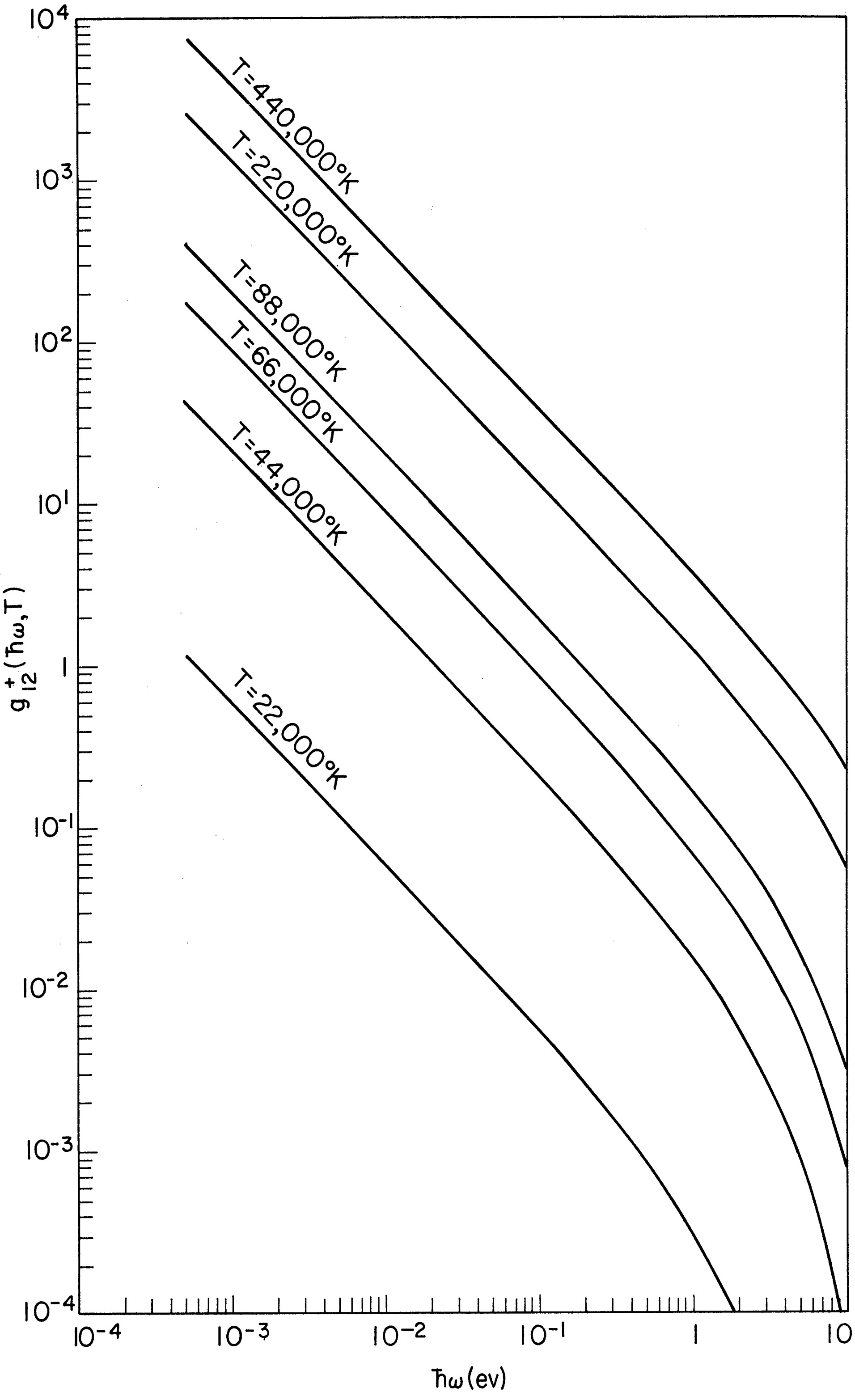

Figure 6a. $g^{+}_{12}(\hbar\omega,T)$.

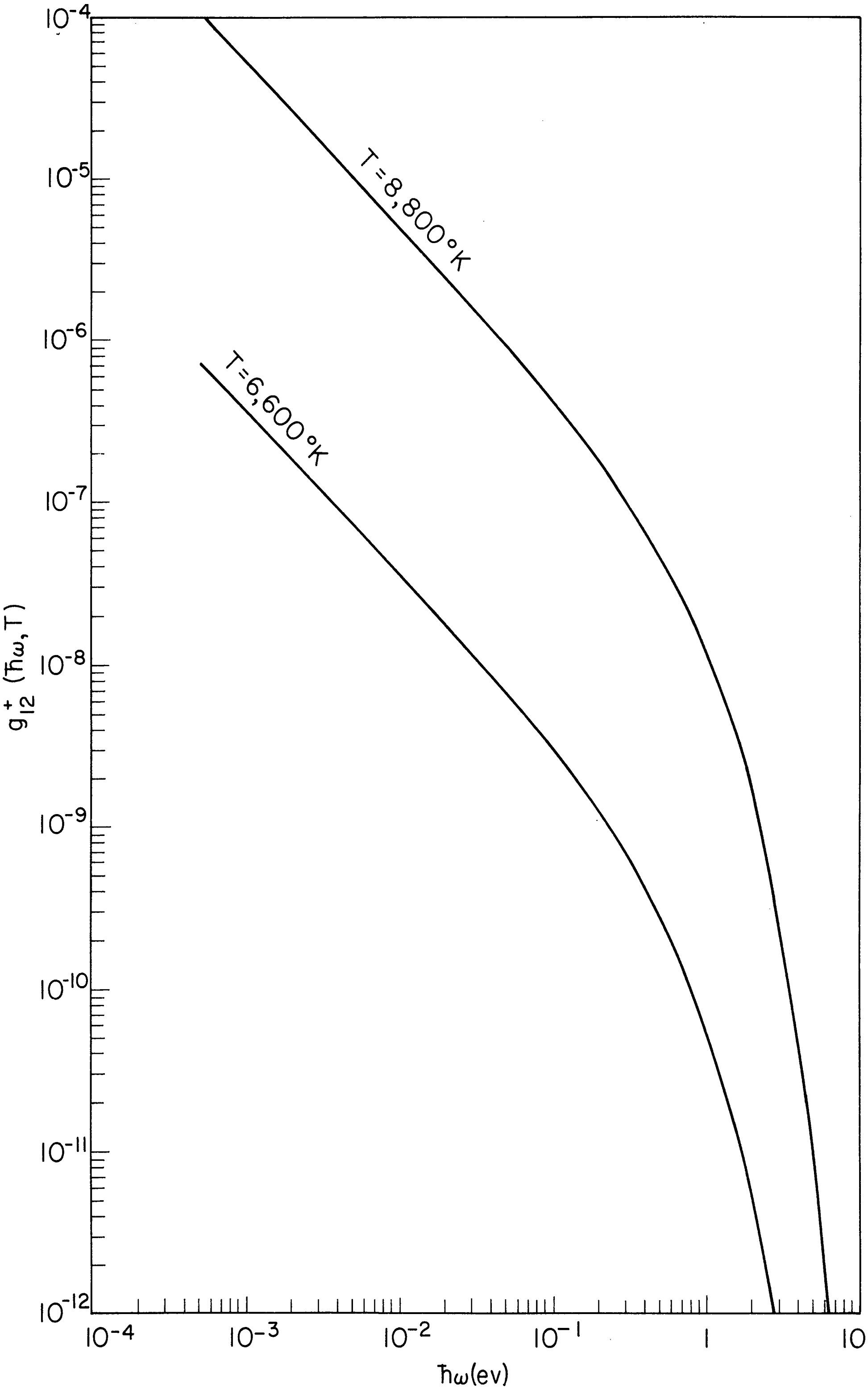

Figure 6b. $g_{12}^{+}(\hbar\omega, T)$.

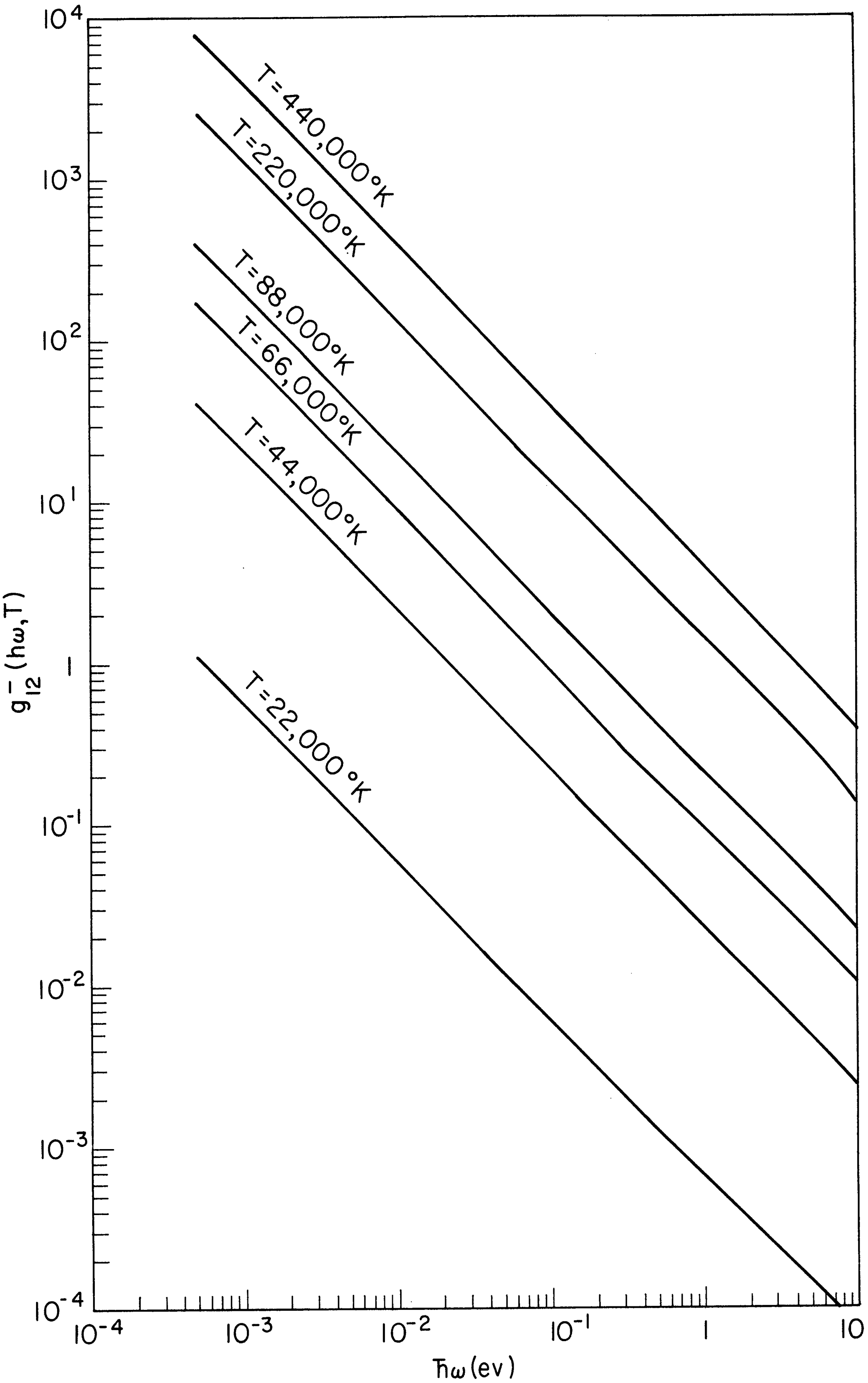

Figure 7a. $g_{12}^-(\hbar\omega,T)$.

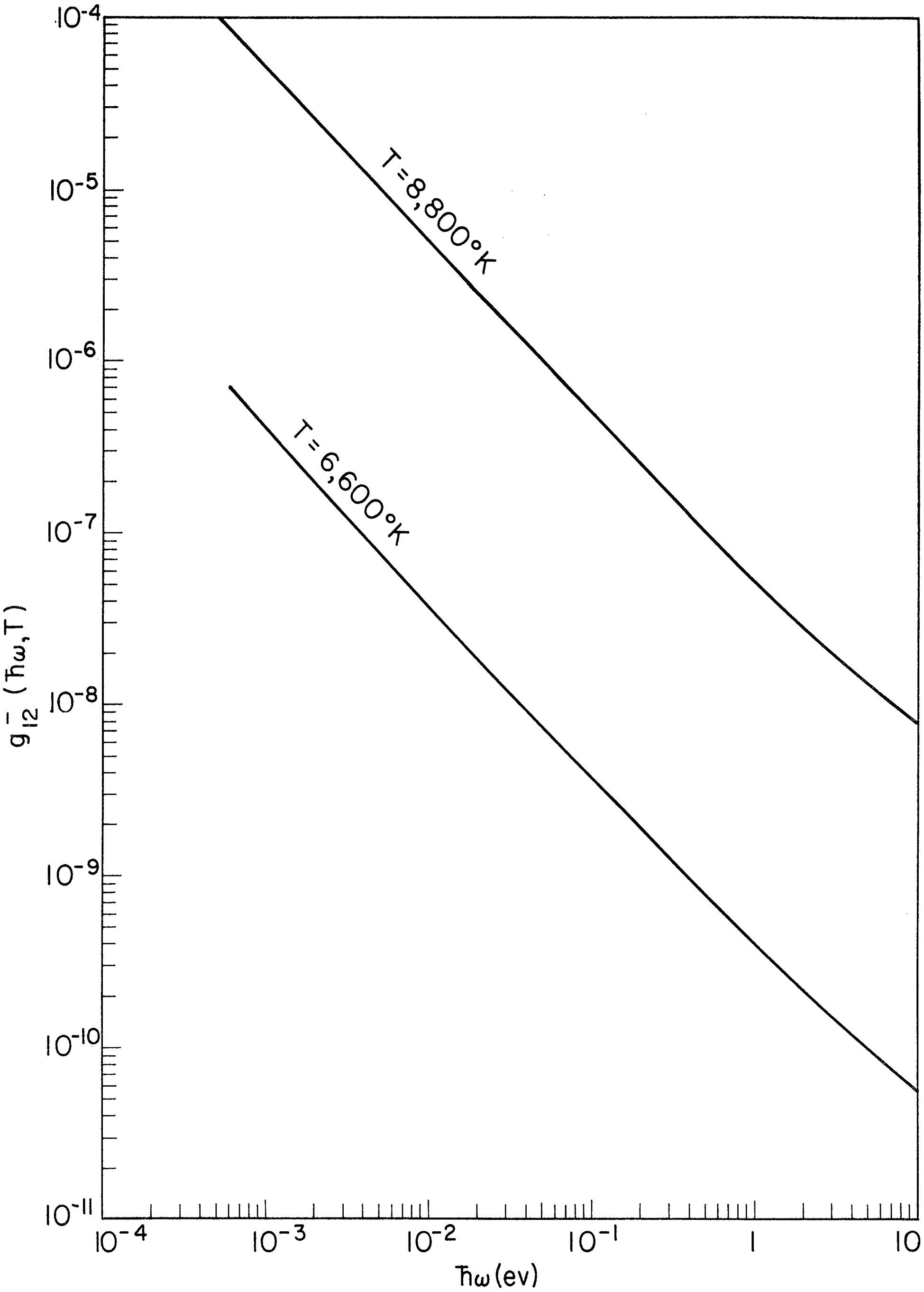

Figure 7b. $g_{12}^{-}(\hbar\omega, T)$.

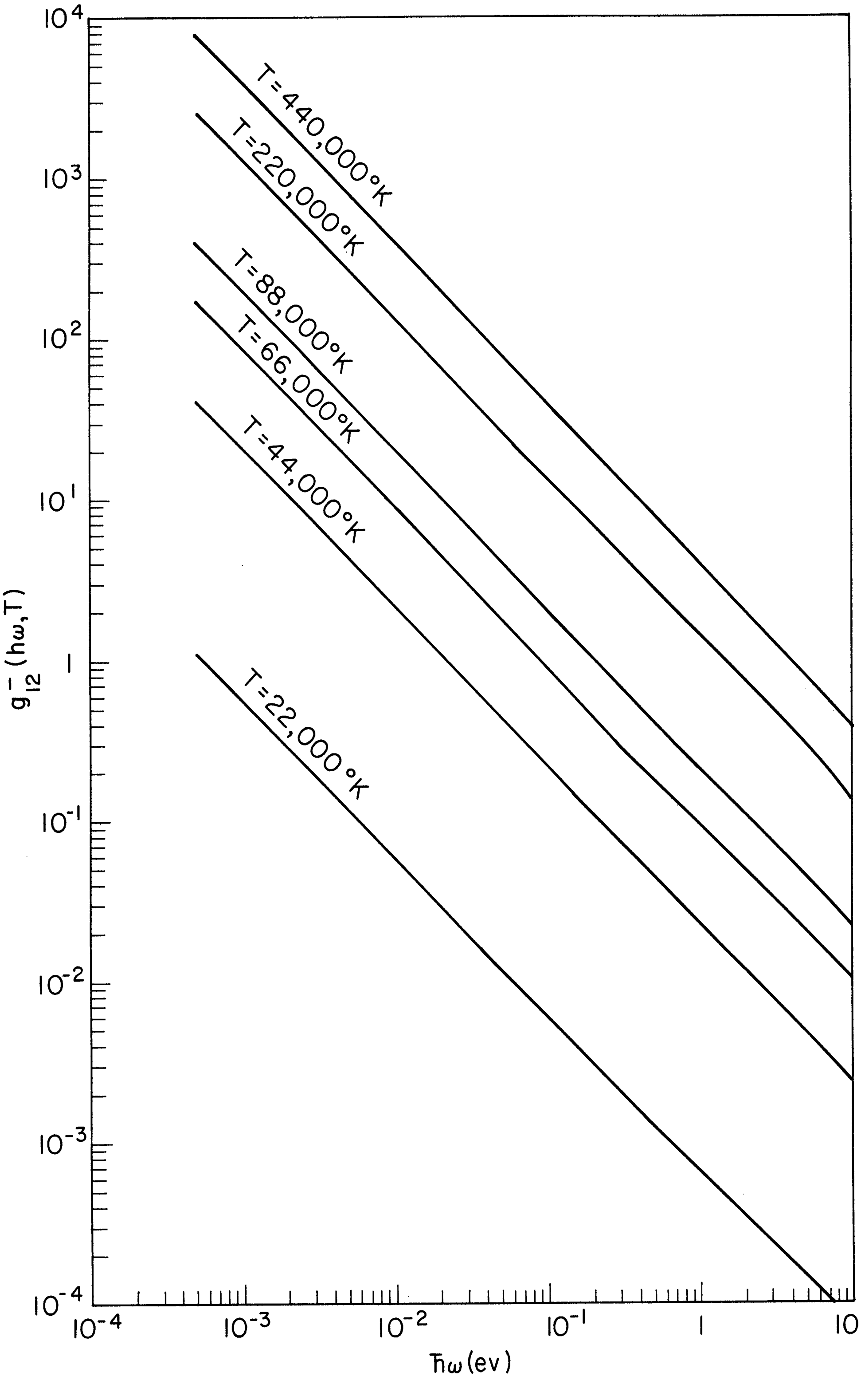

Figure 7a. $g_{12}^{-}(\hbar\omega,T)$.

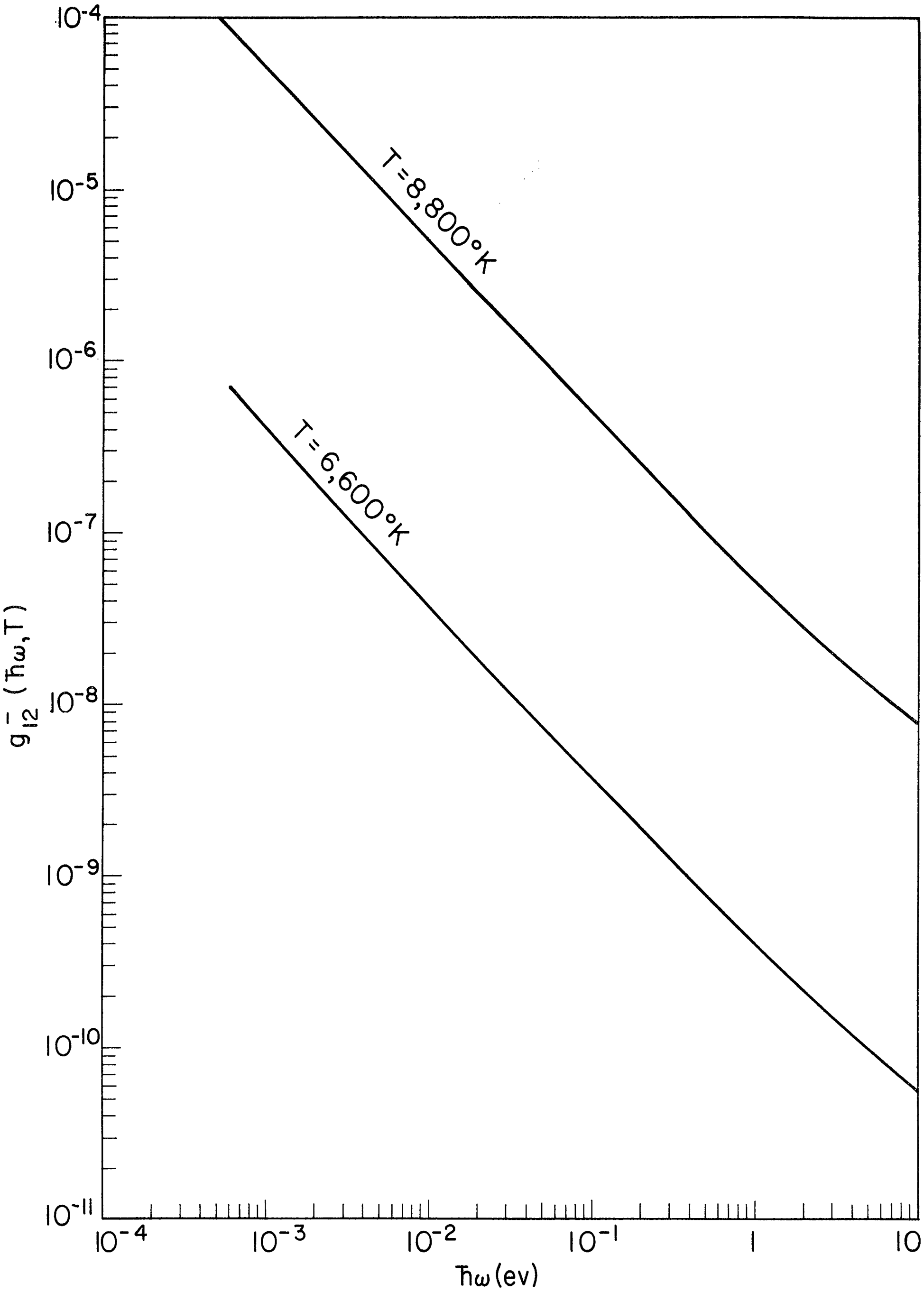

Figure 7b. $g^{-}_{12}(\hbar\omega,T)$.

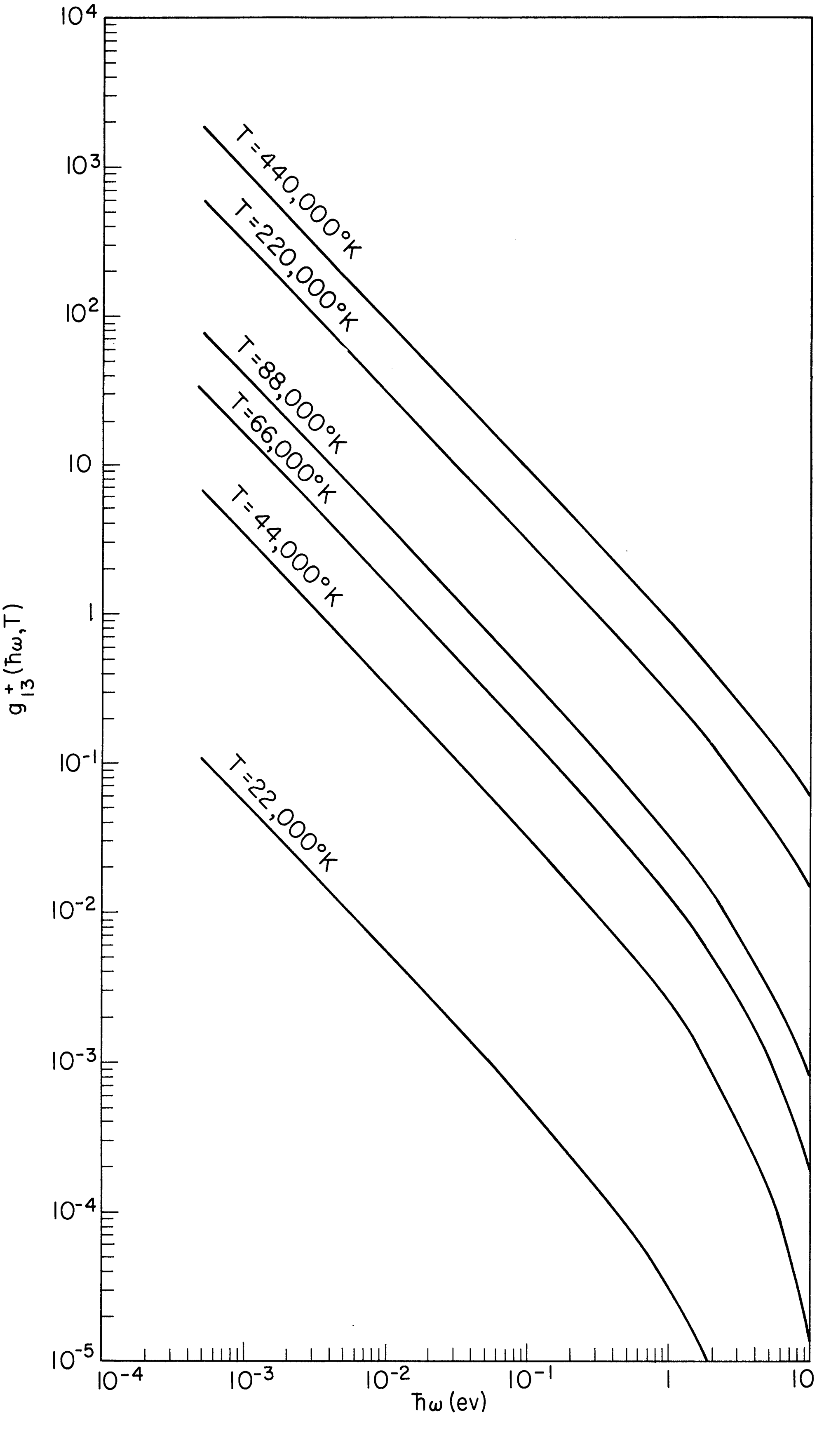

Figure 8a. $g_{13}^{+}(\hbar\omega,T)$.

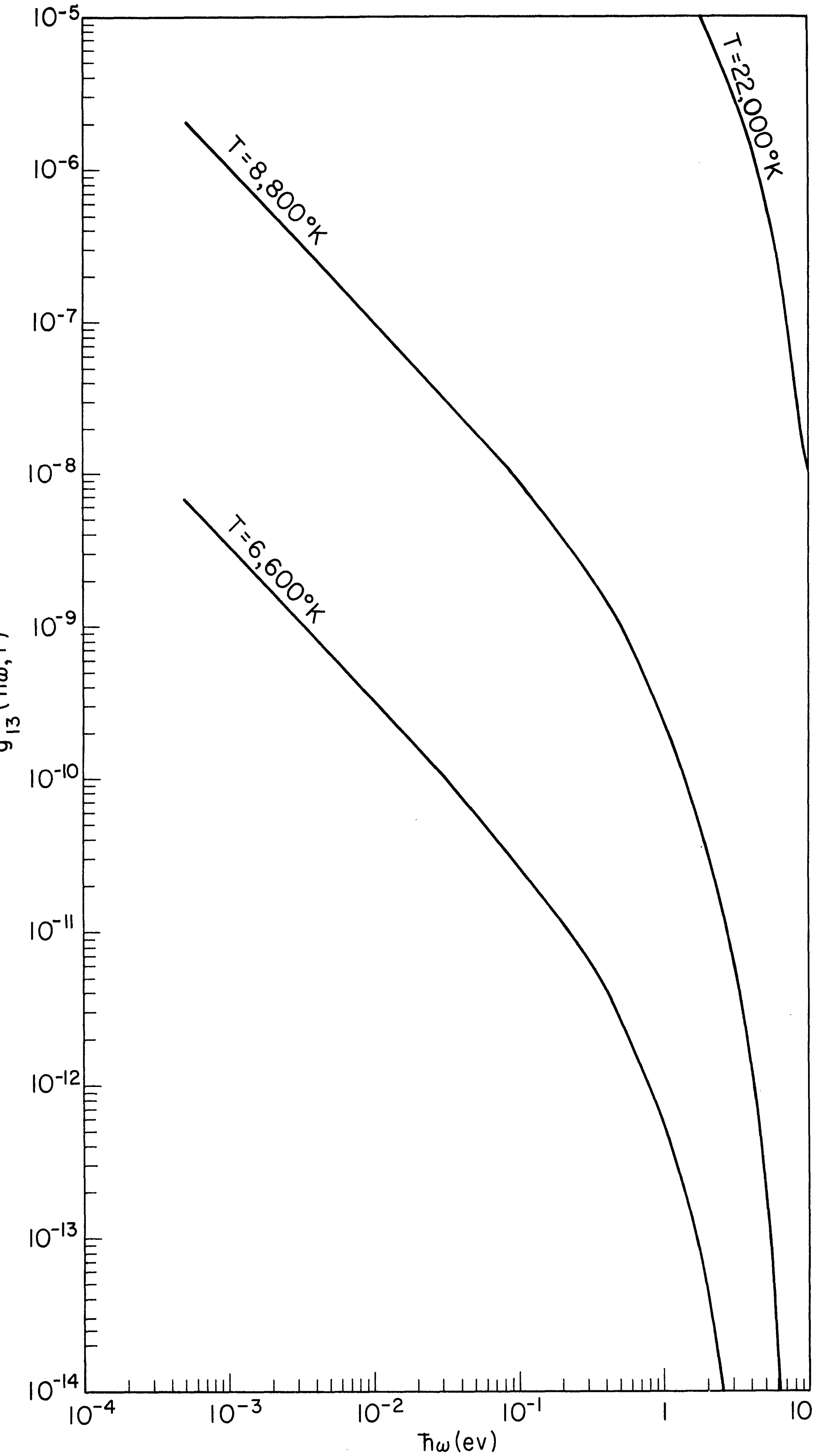

Figure 8b. $g^{\mp}_{13}(\hbar\omega, T)$.

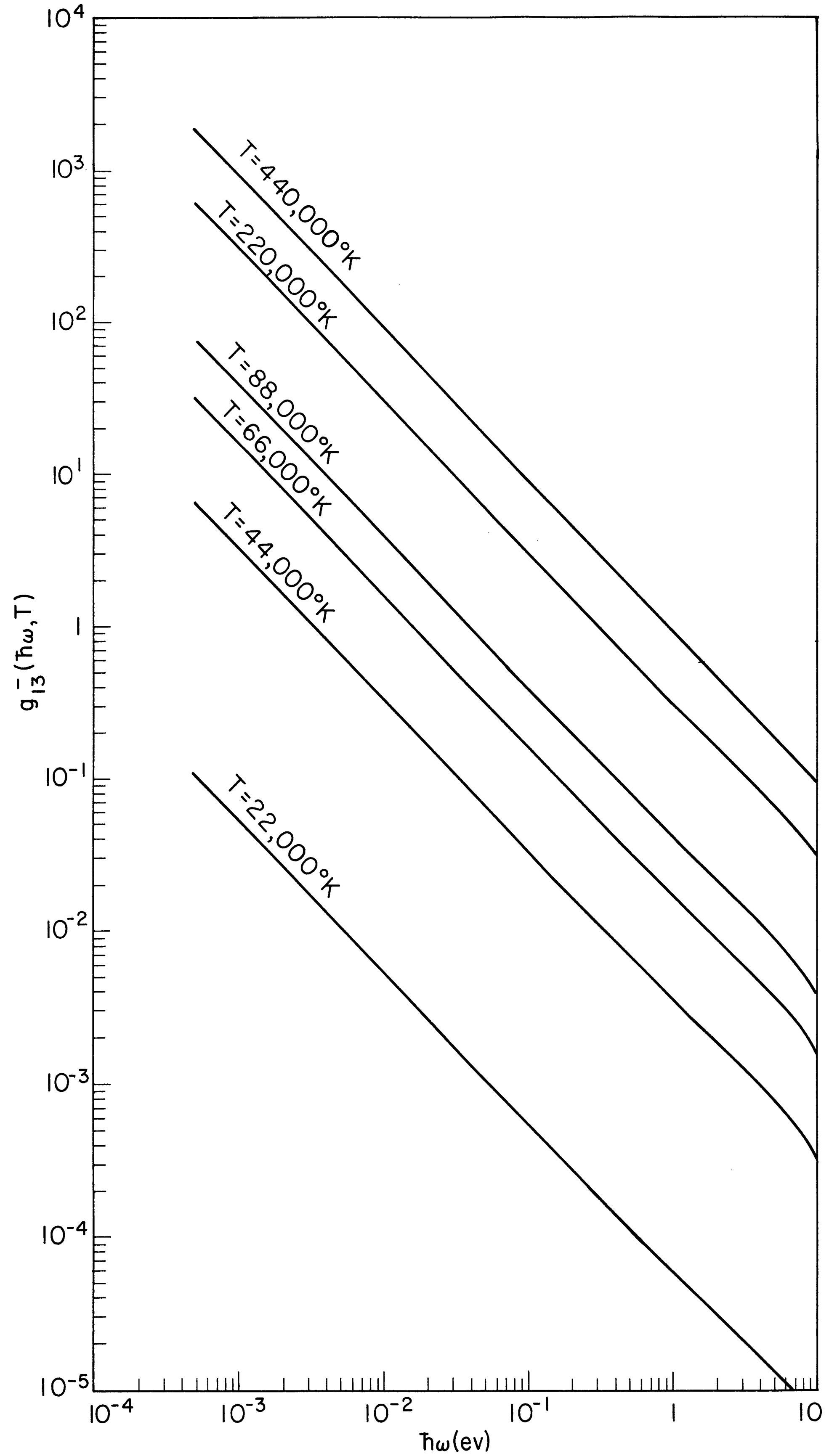

Figure 9a. $g_{13}^-(\hbar\omega, T)$.

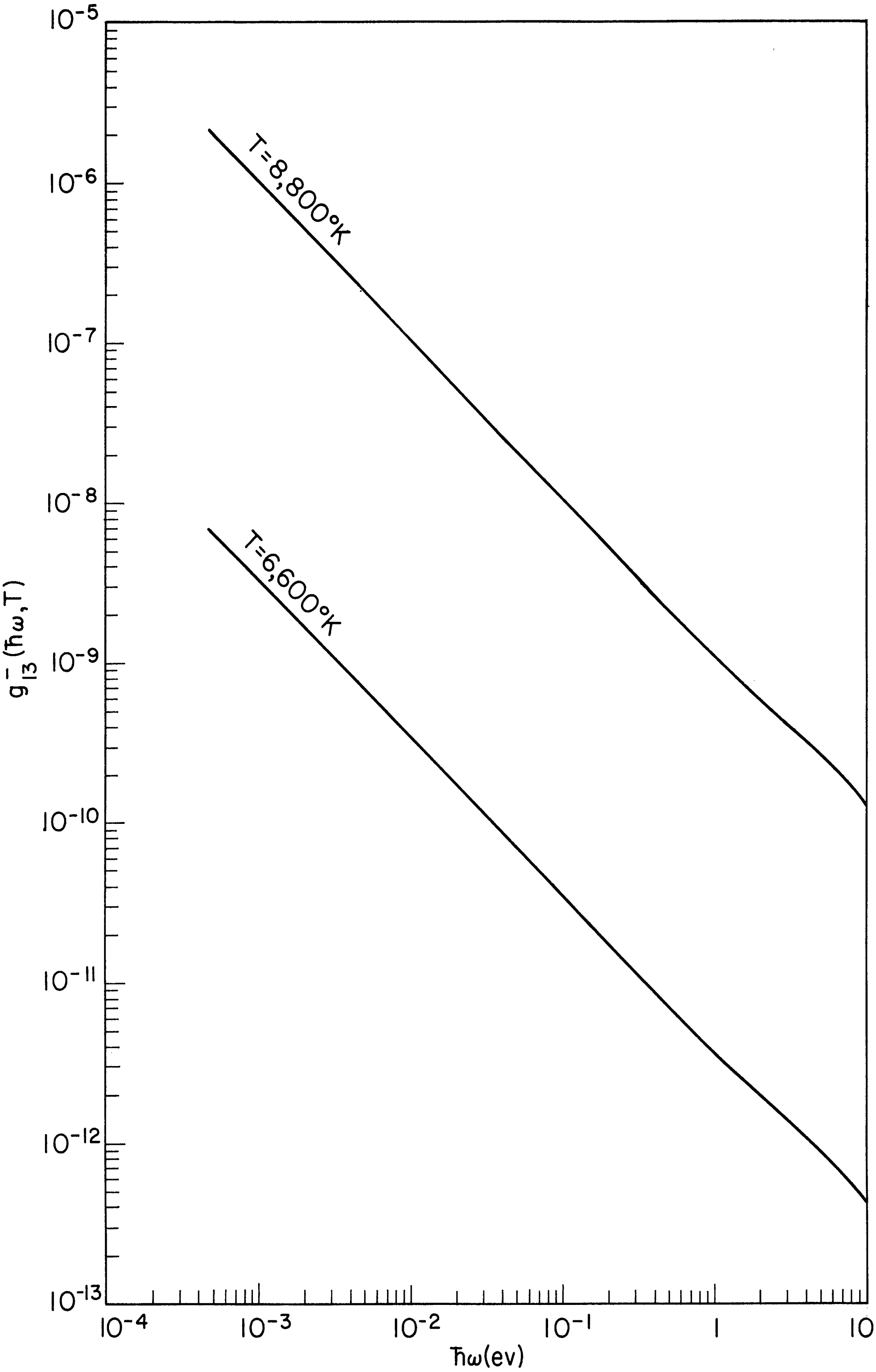

Figure 9b. $g_{13}^{-}(\hbar\omega,T)$.

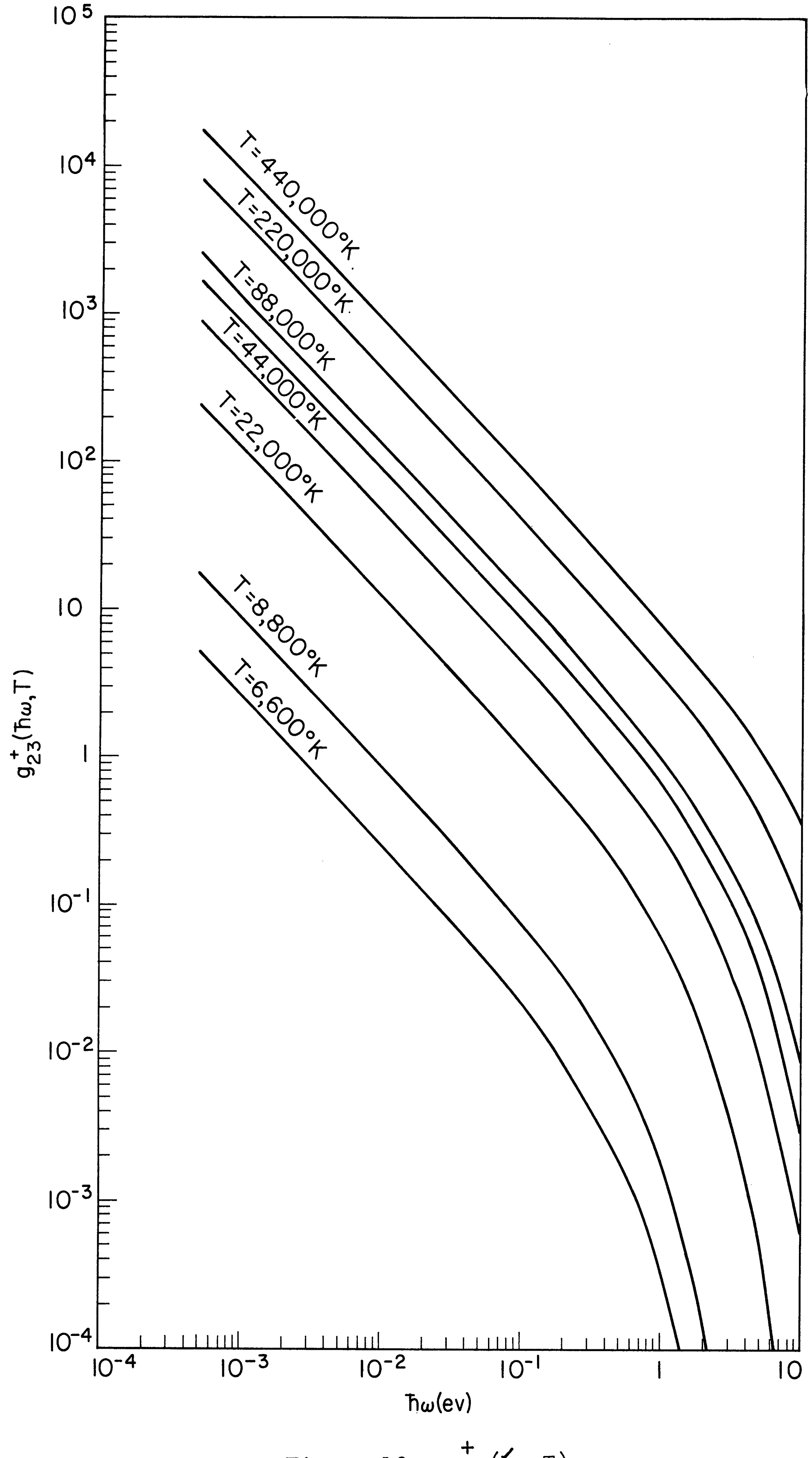

Figure 10. $g_{23}^{+}(\hbar\omega,T)$.

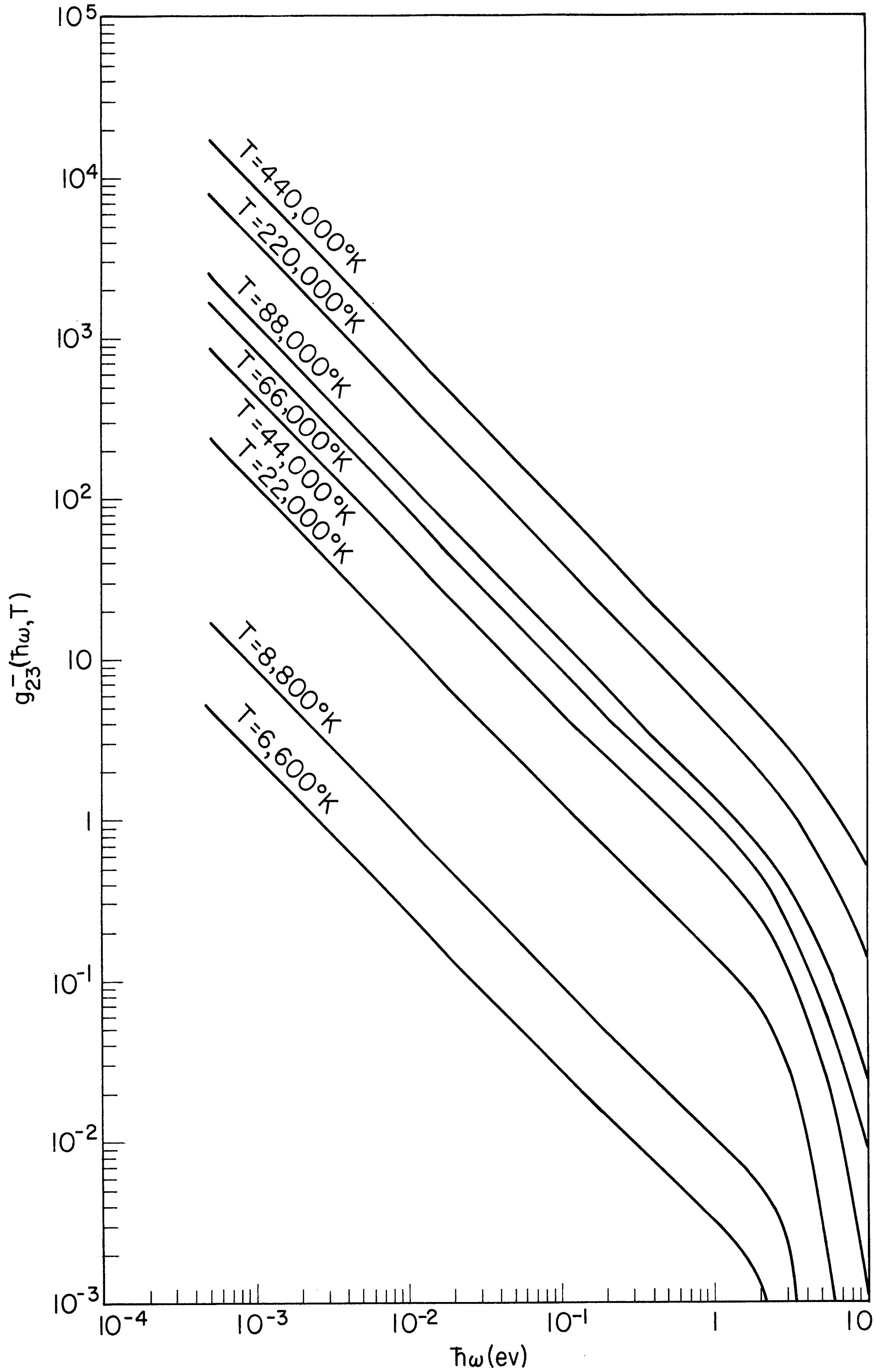

Figure 11. $g_{23}^-(\hbar\omega,T)$.

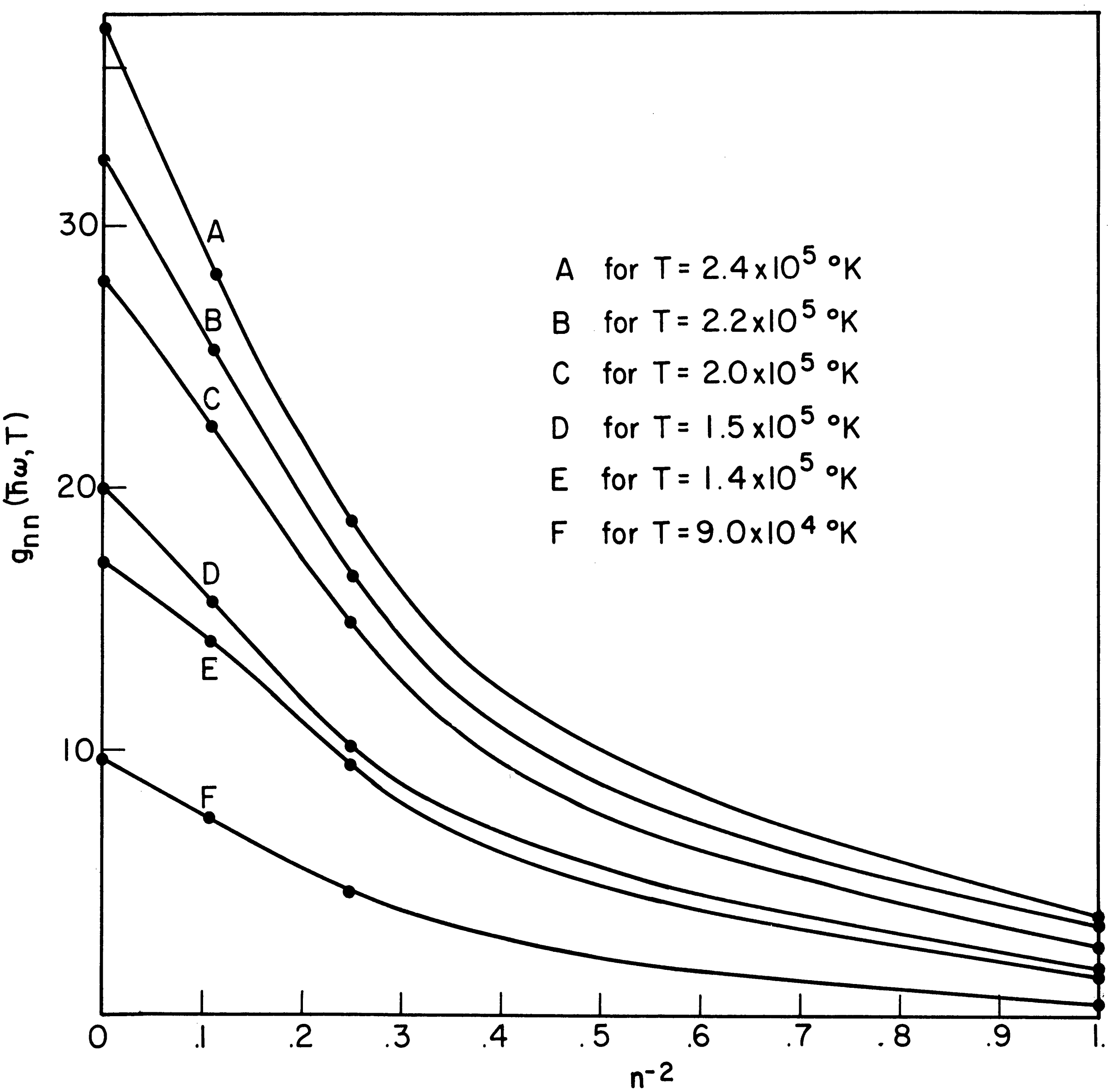

Figure 12. $g_{nn}(\hbar\omega, T)$ vs. $1/n^2$ for ruby laser frequency.

absorption due to $g^{\pm}_{nn'}$ for $n \neq n'$ can be neglected as compared to the contributions due to g_{nn}. With this neglect, the absorption coefficient due to the sum of the contributions in different states is

$$\alpha(\hbar\omega,\Theta) = \sum_n \alpha_{nn}(\hbar\omega,\Theta)$$

$$= c_o(e^{\frac{\hbar\omega}{\Theta}} - 1)\hbar\omega\, N_e \sum_n g_{nn}(\hbar\omega,\Theta)N(n). \quad \text{(IV-51)}$$

With the values of $g_{nn}(\hbar\omega,\Theta)$ determined above, one can obtain from eq. (IV-51) the radiation absorption coefficient due to inverse bremsstrahlung of electrons in the field of hydrogen atoms if the electron density N_e, the neutral densities in the different energy levels $N(n)$ and the temperature of the hydrogen plasma are given.

6. EXPERIMENTAL CONDITIONS AND THE MEASURED ABSORPTION RESULTS

In 1966 Litvak and Edwards[13] measured the absorption coefficient of the ruby laser frequency ($\lambda = 6943$Å) for different initial gas pressures in a hydrogen plasma produced by a giant pulsed laser beam. The output of the laser beam for producing the plasma is $\frac{1}{2}$ - 5 MW peak power with a pulse width of about 18-36 nsec. A 25-cm focal length lens was used to focus the laser output near the center of a brass cubic cell which contains hydrogen gas. The initial gas pressures before the light went in were 14.7, 35, 55, 115, 215, and 1015 psi. Although the initial gas temperature was not mentioned in Litvak and Edwards work, we assume that it was room temperature.

The measurements of the absorption coefficients for the different initial gas pressures were performed at the peak luminosity which occurred near the end of the laser pulse. The electron density and the plasma temperature for each initial pressure corresponding to the absorption measurements were also measured. Table I shows their measured results of plasma temperature T, electron density N_e and absorption $(\alpha L)_{obs}$ for different initial gas pressure p_1. L is the plasma absorption thickness which Litvak and Edwards assumed to be varied from about 1cm for 14.7 psi to 1mm for 1015 psi.

In order to explain the measured absorption results, Litvak and Edwards also calculated the absorption coefficient α_ν from the expression

$$\alpha_\nu = \frac{8}{3(3\pi)^{1/2}} \frac{c^2}{\hbar} (\alpha a_o)^3 \frac{E^{3/2}}{\sqrt{\Theta}\nu^3} N_e^2 \left(g_{ff} + \frac{2E}{\Theta} \sum_n g_{fn} \frac{e^{\frac{E}{n^2\Theta}}}{n^3}\right)\left(1-e^{-\frac{\hbar\omega}{\Theta}}\right) \qquad \text{(IV-52)}$$

which accounts for photoionization and inverse bremsstrahlung of electrons in the field of ions. Eq. (IV-52) is obtained[34] from the absorption coefficient of a hydrogen atom in the energy level E_n due to photoionization and its inverse

$$\alpha_n^{PI} = \frac{64\alpha}{3^{3/2}} \pi a_o^2 \left(\frac{E}{\hbar\omega}\right)^3 \frac{g_{fn}}{n^5} \left(1-e^{-\frac{\hbar\omega}{\Theta}}\right) N(n) \qquad \text{(IV-53)}$$

through the use of Saha equation

$$N(n) = \left(\frac{2\pi\hbar^2}{m\Theta}\right)^{3/2} n^2 \exp\left(\frac{E}{n^2\Theta}\right) N_e^2 \qquad \text{(IV-54)}$$

where g_{fn} is the Gaunt factor for free-bound transitions.[34,35] The calculated α_ν shown in Table I is two orders of magnitude less than the measured result under the assumption that the plasma thickness varies from about 1cm for 14.7 psi to 1mm for 1015 psi. This large descrepancy indicates that the measured absorption can not be explained by the photoionization and the inverse bremsstrahlung of electrons in the field of ions through the use of Saha equation.

In the following sections we propose to explain the absorption which is measured in this experiment by considering the photoionization process and the inverse bremsstrahlung of electrons in the field of neutral atoms. In this explanation we shall not use the Saha equation to predict the number of neutral atoms in the plasma, but rather we shall determine it from an investigation of the explosion caused by the laser pulse.

7. DESCRIPTION OF AN INTENSE POINT EXPLOSION

It was shown by Litvak and Edwards from the consideration of the measured pressure and energy variations with time that the giant laser pulse produces an intense point explosion with a spherical shock wave. The problem for an intense point explosion has been investigated by Sedov.[36] After the energy E^o is absorbed into the gas with initial pressure p_1 and mass density ρ_1 for initiating the explosion, a shock wave forms and expands in the course of time. Sedov defined ρ_2, p_2 T_2 and r_2 as the total mass density, the pressure, the temperature and the radius of a point behind the shock wave at the time t after the explosion. Furthermore,

$$t^{o} = r^{o} \left(\frac{\rho_1}{p_1}\right)^{\frac{1}{2}} \qquad \text{(IV-55)}$$

and

$$r^{o} = \left(\frac{E^{o}}{p_1}\right)^{\frac{1}{3}} \qquad \text{(IV-56)}$$

were defined and Litvak and Edwards called them as the characteristic time and shock radius at which the counter pressure of the undisturbed gas nearly stops the expansion of a spherical explosion. By solving the equations of motion, continuity and energy, one can determine the density, pressure and temperature distributions ($\frac{\rho}{\rho_2}$, $\frac{p}{p_2}$, and $\frac{T}{T_2}$) as functions of $\frac{r}{r_2}$, as well as the pressure and the density behind the shock front ($\frac{p_2}{p_1}$ and $\frac{\rho_2}{\rho_1}$) as functions of $\ell = \frac{r_2}{r^o}$. The symbols ρ,p,T, and r are respectively the density, the pressure, the temperature and the radius of a point between the shock front and the explosion center which depend on time implicitly through $r_2(t)$. Reference (36) contains the graphical representations of the above distributions for the adiabatic index γ=1.4. For our later use and for a quantitative understanding of their variations, we reproduce $\frac{\rho}{\rho_2}$, $\frac{p}{p_2}$, and $\frac{T}{T_2}$ in Figures 13-15. From Fig. 13, one can see that during the early times after explosion, most particles are concentrated behind the shock wave and a negligible amount of particles occupies the central region of the explosion.

In addition, Sedov also obtained the following equations

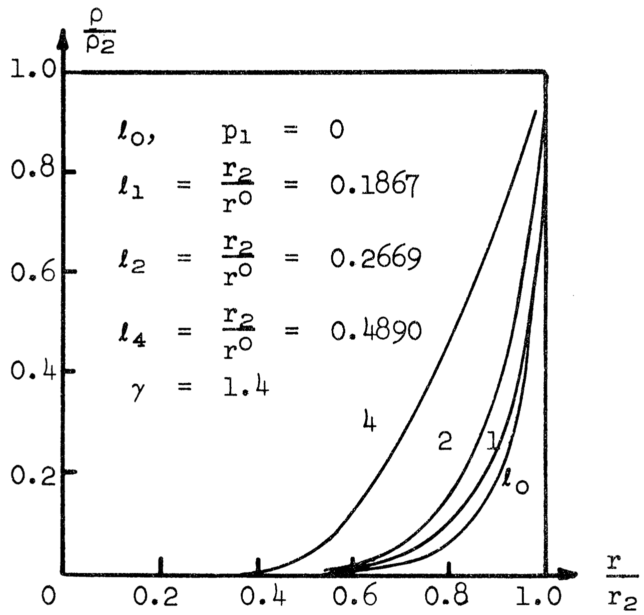

Figure 13. Density distribution in a point explosion behind spherical shock wave.

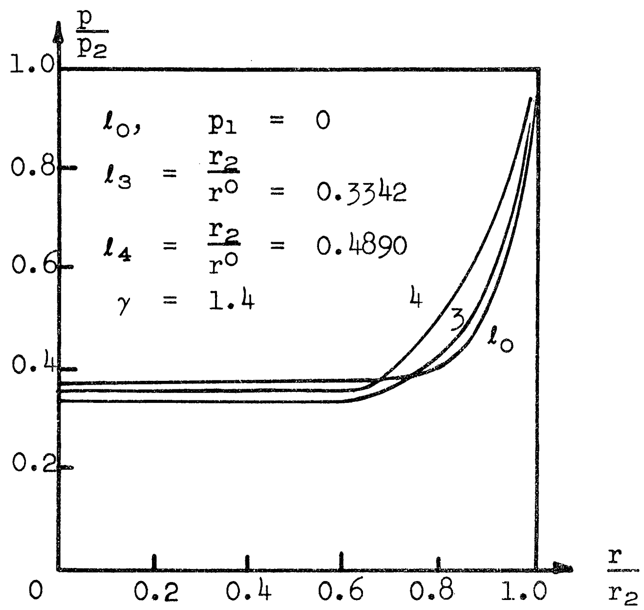

Figure 14. Pressure distribution in a point explosion behind spherical shock wave.

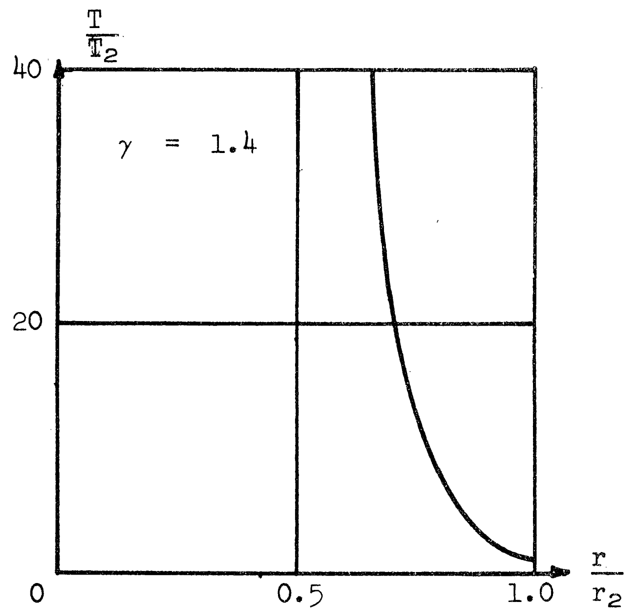

Figure 15. Temperature distribution in a point explosion behind spherical shock wave.

$$\frac{\rho_2}{\rho_1} = \frac{\gamma+1}{\gamma-1+2q}$$

$$\frac{p_2}{p_1} = \frac{2\gamma-(\gamma-1)q}{(\gamma+1)q}$$

$$q = \frac{25}{4}\gamma\frac{\ell^3}{\alpha}$$

$$r_2 = \left(\frac{\alpha E^o}{\rho_1}\right)^{\frac{1}{5}} t^{2/5}$$

for spherical shock wave where q is the square of the ratio of the sound speed in the undisturbed gas to the shock wave velocity. α is a quantity which depends on γ and the shock wave geometry. For the plasma in Litvak and Edwards experiment $\gamma=5/3$, and for a spherical shock wave one can find α from reference (36) as $\alpha=2$. Then one obtains from the above mentioned equations

$$\ell = \frac{r_2}{r^o} = (2\tau^2)^{1/5} \qquad \text{(IV-57)}$$

$$\frac{\rho_2}{\rho_1} = \frac{32}{8+125\ell^3} \qquad \text{(IV-58)}$$

$$\frac{p_2}{p_1} = \frac{240-250\ell^3}{1000\ell^3} \qquad \text{(IV-59)}$$

where $\tau=t/t^o$.

By taking E^o to be the energy absorbed from the laser, Litvak and Edwards obtained the characteristic shock radius r^o from eq. (IV-56) which is given in Table I. The initial mass density ρ_1 and gas pressure p_1 of the plasma are known. We calculated the characteristic time t^o shown in Table I from eq. (IV-55) which checks with the Litvak and Edwards result.

In addition, Litvak and Edwards determined spectroscopically the peak luminous volume. The absorption was measured at the time when the peak luminous volume occurred. Although the luminous volume has been observed to have a nonspherical shape due to the rapid axial motion occurring during the laser absorption, for a quantitative discussion, we shall assume that it has spherical shape and coincides with the shock volume at the instant when the peak luminosity occurred (we shall justify this assumption presently). Then the radius r_2 of the peak luminous volume can be found from its volume. The values of r_2 for each initial pressure are given in Table I together with the corresponding values of $\ell = \frac{r_2}{r^o}$. Under the spherical assumption of the peak luminous volume, r_2 turns to be 0.062cm, much less than 1cm which is assumed by Litvak and Edwards as the absorption length in the plasma. We shall calculate the total absorption using the value of r_2 as obtained above in section IV-8.

In order to justify the above assumption, we now calculate the time t at which the peak luminosity occurs (i.e., the time at which the absorption measurement is taken) from eq. (IV-57) and the value of ℓ corresponding to the peak luminosity volume in Table I. The results are also given in Table I. We observe that t varies between 17-31 nsec. As we mentioned before, the width of the laser pulse varried in the experiment between 18-36 nsec. The early part of the pulse produces the plasma, and according to Litvak and Edwards, the peak luminosity occurs near the end of the pulse. Hence, the values of t calculated above agree reasonably well with the experimental conditions.

Since ℓ is small for the time at which the peak luminosity occurs, the total mass density ρ_2 behind the shock wave, i.e., at r_2, is obtained from eq. (IV-58) to be about four times the initial density ρ_1, as also pointed out by Litvak and Edwards. The pressures p_2 behind the shock wave at the time the peak luminosity occurs, and at the time t=0.1μsec are obtained from eq. (IV-59) and shown in Fig. 16. For comparison, the pressure measured at t=0.1μsec is also shown in the same figure. The measured pressure at t=0.1μsec. is six times the pressure predicted by the explosion theory at the same instant for the initial pressures p_1=14.7 and 35psi. At higher initial pressures, it decreases and reaches about the same pressure as predicted for p_1=1015 psi. If one extrapolates the measured pressures up to the time at which the peak luminosity occurs, a descrepancy is observed between the extrapolated value and the presssure predicted by the point explosion theory for the same instant. Here also, this descrepancy is large for low initial gas pressures and small for high initial pressures. This may indicate that the point explosion assumption is better justified at high initial gas pressures than at low initial pressures. Since the focal volume of the laser beam is elongated in the direction of the beam, and since the energy absorption decreases away from the source due to the attenuation of initial laser beam producing the shock, an egg-shaped shock front is perhaps a more accurate description than the spherical shock front

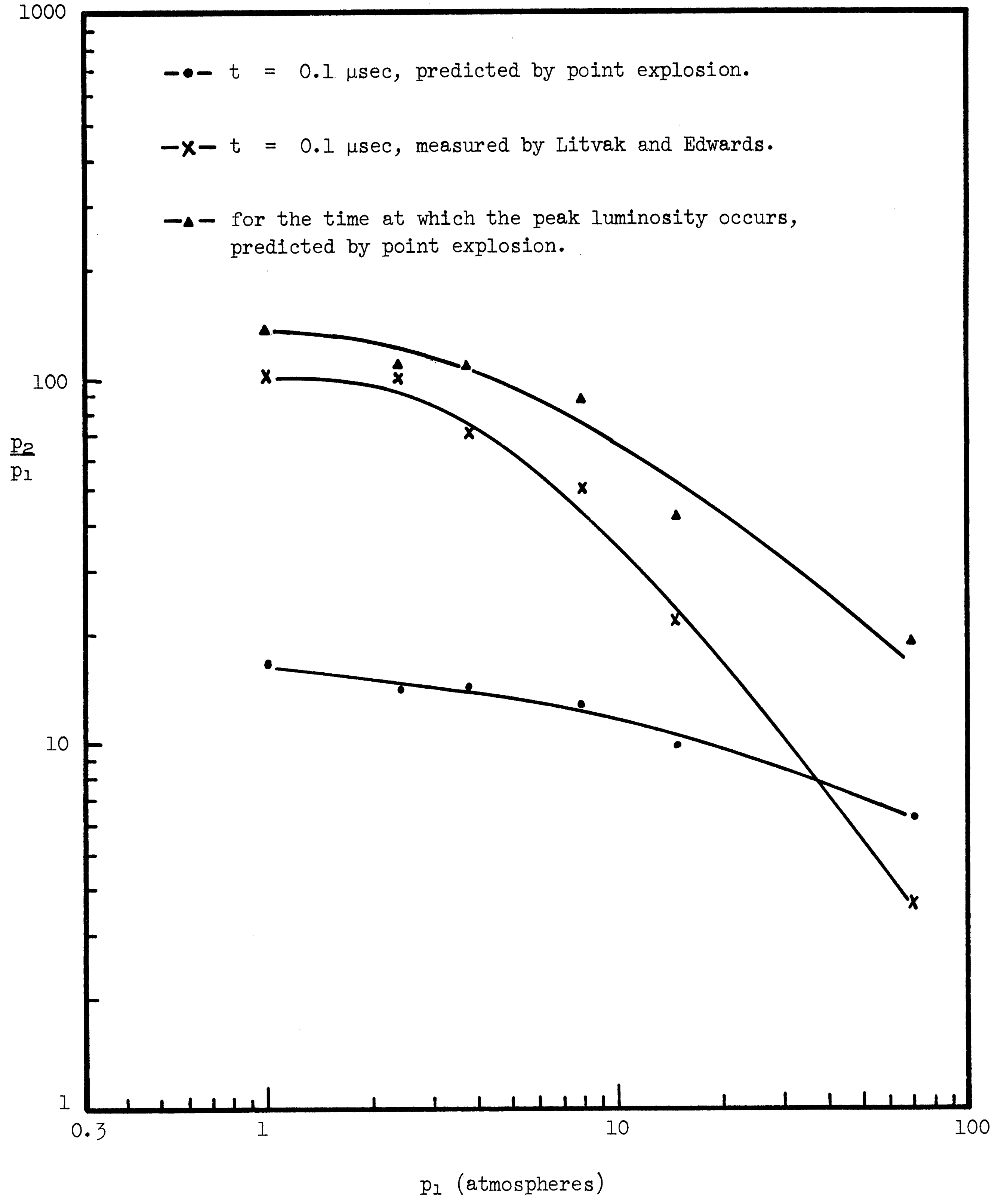

Figure 16. Relative pressure p_2/p_1 behind shock front vs. p_1.

as we assumed above. Furthermore, the initial volume of explosion which can be taken as the focal volume ($10^{-5} cm^3$) of the laser beam is not negligible as compared to the shock volume ($8 \times 10^{-3} cm^{-3}$) even at 0.1 μsec. This may also be a contributing factor to the discrepancy in the measured and calculated pressures.

The point explosion assumption, as pointed above, predicts the location of the shock front reasonably well. Since we need the result of the point explosion theory only to estimate the neutral density distribution within the shock volume and the shock size in our absorption calculations, and since the pressure behind the shock front does not enter our absorption formulas, the above discrepancy in the estimation of pressures is not critical for our purpose.

8. ABSORPTION CALCULATION BASED ON NEUTRAL DISTRIBUTION INSIDE A SHOCK WAVE

In this section, we shall calculate the absorption due to the photo-ionization process and the inverse bremsstrahlung of electrons in the field of neutral atoms by using the particle distribution inside a shock wave, i.e., Fig. 13. In doing this, one has to determine first the population of the excited levels of the hydrogen atoms as a function of position in the plasma. We assume local thermal equilibrium among the neutral atoms, i.e., eq. (IV-44) so that the relative populations of the excited levels is not an explicit function of position (it may depend on position through temperature). Then the local absorption coefficient due to the inverse bremsstrahlung of electrons in the field of neutrals can be written

$$\alpha^{BN}(r) = \sum_{n=1}^{n^*} A_n(\omega,\Theta)\, N_e(r)\, N(1,r)\, \frac{N(n)}{N(1)} \tag{IV-60}$$

where $N(n)/N(1) = n^2 e^{-E_n|\Theta}$ and $A_n(\omega,\Theta)$ is a function of temperature and radiation frequency. $A_n(\omega,\Theta)$ increases with n, approaching finite value $A_\infty(\omega,\Theta)$ as $n\to\infty$. Since $E_n \to E$ as $n\to\infty$, the above summation diverges unless it is truncated at some $n=n^*$. The physical reason for truncating the summation at some $n=n^*$ can be explained as follows: Because of the interaction of an atom with the nearby particles in a plasma, the ionization potential will be lowered when the atom is inside a plasma. An excited atom in a level above n^* must be treated as an ion and a free electron even though the level may be below the ionization potential of an unperturbed atom. Several theories for the determination of n^* and the lowering of the ionization potential ΔE have been proposed in literature. Drawin and Felenbok[37] have reviewed these theories and showed that they all yield similar results, i.e.,

$$n^{*2} \approx (S+1)\,\frac{\rho_D}{a_o} \tag{IV-61}$$

$$\Delta E \approx (S+1)\,\frac{e}{\rho_D} \tag{IV-62}$$

where ρ_D is the Debye radius[38,39] given by

$$\rho_D = \left[\frac{kT}{4\pi e^2 (N_e + \sum_i z_i^2 N_i)}\right]^{1/2} \tag{IV-63}$$

In eqs. (IV-61) and (IV-62), S is the ionization stage of the particle under consideration and S=0 for neutral atoms. The quantities N_i and z_i in eq. (IV-63) are respectively the density and charge of neighboring ions and for hydrogen plasma, $z_i=1$ and $N_i=N_e$. We have calculated and tabulated in Table I the values of n* for each initial gas pressure using the measured electron density and temperature in the experiment by Litvak and Edwards.

After having determined n* in eq. (IV-60), we now consider the position dependence of the number density in eq. (IV-60). According to the intense point explosion theory, the relative mass density distribution follows the curves in Fig. 13 for the early times after explosion. One observes that the particles occupy vitually a very narrow spherical shell of a thickness of the order of 0.2 r_2. We shall refer to this region as the shell region in below. The central region contains very few particles. However, the temperature increases very rapidly in this region towards the center and the pressure is constant with a value of approximately $p_2/3$. We shall refer to this region as the central hot core. Let the relative number density of the atom at the point r between the shock wave and the explosion center be $\varphi(r)=N(r)/N_2$ and the relative electron density at the point r be $\varphi_e(r)=N_e(r)/N_e$ where $N(r) = \sum_{n=1}^{n^*} N(n,r)$ and N_2 and N_e are respectively the total neutral density behind the shock front and the average electron density inside the shock volume. From the conservation of the particles

$$4\pi \int_0^{r_2} dr r^2 [N_2\varphi(r)+N_e\varphi_e(r)] = \frac{4\pi}{3} r_2^3 N_1$$

where N_1 is the total number density of hydrogen atoms before the explosion (i.e., before the incidence of the laser beam) and r_2 is the radius of the shock wave. After changing the variable, we have

$$\int_0^1 dx x^2 \varphi(x) = \frac{N_1}{3N_2} - \frac{N_e}{N_2} \int_0^1 dx x^2 \varphi_e(x) \qquad \text{(IV-64)}$$

and

$$3\int_0^1 dx x^2 \varphi_e(x) = 1 \qquad \text{(IV-65)}$$

where

$$x = \frac{r}{r_2} .$$

The laser beam was focused within a volume of 10^{-5} cm^3 which is smaller than the peak luminous volume of 10^{-3} cm^3 at the time of the absorption measurement. The radius of the laser beam focal volume is about 5 times less than the radius of the peak luminous volume. No geometry correction is needed in determining the optical path. Hence the absorption due to the inverse bremsstrahlung of electrons in the field of neutral atoms can be expressed, by introducing the relative number densities into eq. (IV-60), as

$$(\alpha L)^{BN} = \sum_{n=1}^{n*} \int_{-1}^{1} dx A_n(\omega,\Theta) N_e N_2 \frac{N(n)}{N} r_2 \varphi_e(x)\varphi(x) . \qquad \text{(IV-66)}$$

Equation (IV-66) cannot be easily calculated without any assumption about $\varphi_e(x)$, $\varphi(x)$ and the temperature distribution. The problem will be complicated when the temperature distribution (see Fig. 15) in the shock wave as a function of position is considered. The plasma temperature and the electron density are measured through the line broadening of H_α which depends upon the electron and neutral densities. Since most of the hydrogen atoms are confined in the shell region behind the shock front, the electron density and the plasma temperature measured through the line broadening is more likely to indicate the average temperature and electron density in the shell region. Furthermore, the degree of ionization is not uniform in the shock volume. Due to the very high temperatures, the hydrogen gas can be expected to be fully ionized in the hot core. However, the degree of ionization is more likely to decrease towards the shock front because the temperature there is of the order of 10^4 °K and thus not sufficient for ionization. One may conclude from this argument that the electron density will also be a decreasing function of the radius. However, the rapid increase in the particle density towards the shock front may result in a uniform electron density distribution in spite of the decrease in the degree of ionization. Hence we shall assume that the temperature and the electron density are uniform in the shell region with the measured values.

The contribution to the absorption in the hot core where we expect almost full ionization is negligibly small as compared to the measured absorption. The mechanisms responsible for photon absorption in this region are the inverse bremsstrahlung of electrons in the field of ions and the photoionization. In fact, since the gas is almost fully ionized, the relative contribution of the photoionization process is small as compared to the inverse bremsstrahlung of electrons in the field of ions. Litvak and Edwards calculated the absorption in this region using the measured electron density and temperature, and assuming the Saha equation in estimating the neutral density. Even if one assumes a plasma thickness of 1cm, their result accounted only one percent of the measured absorption. But according to explosion theory the size of the hot core is of the order of 0.12cm. so that the absorption is less than 0.1% of the measured value.

We thus calculate that the main absorption takes place in the shell region where the gas is partially ionized. Under these assumptions, eq. (IV-66) becomes

$$(\alpha L)^{BN} = \sum_{n=1}^{n^*} A_n(\omega,\Theta) N_e N_2 \frac{N(n)}{N} r_2 \int_{-1}^{1} dx\varphi(x), \qquad \text{(IV-67)}$$

where we include the hot core also for convenience even if its contribution is small. The neutral density distribution $\varphi(x)$ is shown in Fig. 13 and has an appreciable value only for x close to 1. It is sufficient for our purpose, but not necessary, to approximate

$$\int_0^1 \varphi(x)dx \simeq \int_0^1 \varphi(x)x^2 dx = \frac{N_1-N_e}{3N_2}$$

Then eqs. (IV-67) reduces, in view of eq. (IV-51), to

$$(\alpha L)^{BN} = \frac{2}{3} c_0 \hbar\omega \left(e^{\frac{\hbar\omega}{\Theta}} - 1 \right) r_2 \frac{N_1-N_e}{z} N_e \sum_{n=1}^{n^*} g_{nn} 2n^2 e^{-E_n/\Theta} \qquad \text{(IV-68)}$$

where

$$z = \sum_{n=1}^{n^*} 2n^2 e^{-E_n/\Theta}$$

is the truncated partition function of hydrogen atom with the calculated

TABLE I

MEASURED AND CALCULATED ABSORPTIONS FOR RUBY LASER FREQUENCY IN THE HYDROGEN PLASMA

p_1(psi)	14.7	35	55	115	215	1015
T(°K)	2.2×10^5	2.0×10^5	2.4×10^5	1.5×10^5	1.4×10^5	9.0×10^4
N_e(cm.$^{-3}$)	4.5×10^{18}	10^{19}	5×10^{18}	10^{19}	8.5×10^{18}	10^{19}
t°(μsec.)	4.9	4.3	4.3	4.0	3.2	1.7
r°(cm.)	0.52	0.46	0.46	0.43	0.34	0.18
r_2(cm.)	0.062	0.062	0.062	0.062	0.062	0.042
ℓ	0.12	0.13	0.13	0.14	0.18	0.23
t(nsec.)	17	18	18	21	31	27
n*	14	12	14	11	11	10
N_1-N_e(cm.$^{-3}$)	4.9×10^{19}	1.2×10^{20}	2.0×10^{20}	4.1×10^{20}	7.7×10^{20}	3.7×10^{21}
z	998	598	1062	362	337	140
α_ν(cm^{-1})	0.012	0.011	0.020	0.15	0.12	0.6
(αL)obs.	0.72	0.80	1.94	3.0	2.64	4.12
$(\alpha L)^{BN}$	0.015	0.087	0.062	0.47	0.75	4.9
$(\alpha L)^{PI}$	0.047	0.20	0.18	1.13	2.26	14.9
$(\alpha L)^{BN+PI}$	0.062	0.29	0.24	1.60	3.01	19.8

values given in Table I.

In a similar way, one can obtain the absorption due to the photoionization and its inverse from eq. (IV-53) as

$$(\alpha L)^{PI} = \frac{128}{3^{5/2}} \pi a_o^2 \left(\frac{E}{\hbar\omega}\right)^3 \left(1-e^{-\frac{\hbar\omega}{\Theta}}\right) r_2 \frac{N_1-N_e}{z} \sum_{n=1}^{n^*} \frac{2g_{fn}}{n^3} e^{-E_n/\Theta} . \quad \text{(IV-69)}$$

Taking r_2 as the radius of the peak luminous volume which is assumed to be spherical, we have calculated the absorptions $(\alpha L)^{BN}$ and $(\alpha L)^{PI}$ from eqs. (IV-68) and (IV-69). The results are given in Table I together with their sum $(\alpha L)^{BN+PI}$.

9. DISCUSSIONS

From Table I, one can see that the calculated absorptions $(\alpha L)^{BN+PI}$ due to the photoionization and the inverse bremsstrahlung of electrons in the field of neutron atoms are not always in good agreement with the measured result $(\alpha L)_{obs}$. It increases from the value of ten times less for P_1=14.7 psi to the value of five times larger for p_1=1015 psi than the measured absorption. According to the description given by Litvak and Edwards, the shape of the luminous volume was not exactly spherical. Although their description was not explicit enough for their experiment, they referred to other similar experiments in which the cigar-shaped or egg-shaped luminous regions were observed in the direction of the laser beam. Furthermore, the discrepancy between the measured pressure and that predicted by the intense point explosion theory with a spherical shock wave is larger at low initial gas pressure than at high pressure. This may suggest that the shape of the shock volume at low initial gas pressure deviates more from spherical at high initial pressure. If we intepret r_2 as the major radius of the luminous volume, then we may predict a larger absorption than we calculated by using a spherical luminous volume. In fact, this may be the reason why Litvak and Edwards assumed the absorption thickness of 1cm for p_1=14.7 psi. If this assumed absorption thickness is correct, r_2 would be 0.5cm, instead of 0.062cm, and the calculated absorption with r_2=0.5cm will be almost the same as the measured value at p_1=14.7 psi, provided that the neutral density distribution along the major axis has a similar distribution to that in the spherical case shown in Fig. 13. At any rate, our interpretation predicts the absorption better than a factor 10, in fact in most cases even better than a factor of 6. Furthermore, our calculation explains the increase of the absorption with the initial pressure, independently of the possible dependence on the pressure of the apparent plasma size.

Another factor which may be contributing to the above discrepancy is the assumption of a uniform temperature and electron density distribution in the shell region behind the shock front. However, the error due to this assumption is not expected to be significant, because we have found only a decrease by a factor of 2/3 assuming a linear electron density distribution in the shell region and taking the electron density to be zero at the shock front.

The calculated absorption due to the photoionization and its inverse is about three times the absorption due to the inverse bremsstrahlung of electrons in the field of neutral atoms for n^* = 10. It depends on n^*.

For small n^*, its contribution is dominant and for large n^* it is negligible as compared to the inverse bremsstrahlung of electrons in the field of neutral atoms. Furthermore, photoionization can occur only for the levels above and equal to n such that $E-E_n \leq \hbar\omega$ and the absorption due to this process varies as $1/_{n}5$. For low energy photons, such as the carbon dioxide laser ($\lambda=10.6\times10^{-4}$ cm, $\hbar\omega=0.117$ev), its contribution will be negligibly small as compared the absorption due to the inverse bremsstrahlung of electrons in the field of neutral atoms.

The absorption per electron and per neutral atom in any level n due to the inverse bremsstrahlung of electrons in the neutral atoms is smaller than the absorption per electron and per ion due to the inverse bremsstrahlung of electrons in the ions as indicated in Fig. 12. They are of the same order of magnitude for almost all n and becoming equal when $n\to\infty$. The relative importance of these two mechanisms depends on the ratio of the neutral to ion densities N_A/N_i. If N_A/N_i is a large number, the inverse bremsstrahlung of electrons in the field of neutral atoms is important, otherwise it is small.

CHAPTER V

CONCLUDING REMARKS

In the first part of this thesis we have compared the photon transport theory in dispersive media to the Maxwell's wave theory by considering the index of refraction and the photon absorption per unit time as well as per unit length. In the photon transport theory the effect of the medium is taken into account by assigning a different frequency to photons of a given wave number in the medium, than their frequency in vacuum. It is implied in this theory that the wave number is the same in the medium and in vacuum.

In Maxwell's theory, the effect of the medium is characterized by a functional which relates the macroscopic current to the electric field. When linearized, this functional is completely defined by the conductivity tensor in the transformed $(\underline{k},s)$ domain. The conductivity tensor is obtained quite generally by using Kubo's linear response theory in terms of the microscopic currents. Thus, we can calculate the index of refraction and the damping coefficient both in time and space in the framework of the Maxwell's theory first in terms of conductivity and then in terms of the microscopic currents with Kubo's theory. In other words, we can express the above observable macroscopic quantities, in terms of microscopic quantities through the Maxwell's equations which describe the electromagnetic phenomena in arbitrary media macroscopically.

It is at this stage one can compare the photon transport theory to the

Maxwell's wave theory, because in the former the index of refraction and the damping coefficient both in time and space are expressed in terms of the microscopic currents.

Following the above procedure, we have found that both theories yield the same results for the index of refraction and the damping coefficient per unit time only in the weakly absorbing media. When the medium is strongly absorbing, the results look quite different although we have not estimated the difference numerically in specific problems.

As to the damping in space, the expressions obtained from the two theories for the index of refraction and the damping coefficient per unit length are similar only if the medium is both weakly absorbing and slightly dispersive. More explicitly, the damping coefficient per unit length is obtained in a weakly absorbing medium (i.e., $n_1 \ll n_o$) as $\frac{4\pi}{n_o c}\, \sigma_\lambda^R(n_o k, \omega_o)$ and $\frac{4\pi}{n_o c}\, \sigma_\lambda^R(k, \frac{\omega_o}{n_o})$ respectively in the Maxwell's theory and the transport theory. Clearly if $n_o \approx 1$, the results are identical.

We feel that a better correspondence between the transport and wave approaches in regard to the damping in space can be established if the photons are dressed such that the frequency is required to be the same but the wave number is allowed to be different in the medium. More research in this direction seems to be called for.

The radiation absorption due to inverse bremsstrahlung of electrons in the field of neutral atoms is formulated by using free electron wave functions. In this approximation, the calculations involving atom-electron cross sections turn out to be identical to the use of the first Born approximation. The elastic cross section for hydrogen atoms in the ground state calculated in Born approximation is less than the cross section calculated from the partical wave method. This discrepancy is large at specially low electron energies. Since the elastic cross section predicted by the partial wave method is in good agreement with the experiment, a more accurate formulism of the absorption problem can be achieved by using the partial wave method rather than plane waves. However, since the elastic and inelastic collisions of electrons with the atoms in excited states are also involved in the problem, the use of the partial wave method would make the problem much too complicated. Undoubtedly, the use of free electron wave functions in the problem will introduce some error, perhaps predicting smaller values for the absorption. However, at this stage, one is satisfied with an order of magnitude agreement between the measured and calculated absorptions due to the uncertainties of the experimental condition. This justifies the approach we have taken in this work.

In the formulation of the radiation absorption, the second quantization is used to express the potential between atom and electron as well as the interaction between particle and radiation in terms of the particle and radiation creation and destruction operators. In this process we considered only the binary collisions. In addition, we assumed the atoms in the medium to be infinite heavy. These assumptions are adequate for our stated purpose in this thesis.

The neutral density determined through the Saha equation (which holds when all the particles are in local thermal equilibrium) and using the measured electron density and temperature in Litvak and Edwards experiment is about three orders of magnitude less than the initial particle density. The absorption calculated by Litvak and Edwards in considering only the photoionization and the inverse bremsstrahlung of electrons in the field of ions through the use of Saha equation is negligible as compared to the measured result.

According to intense point explosion theory, most particles are concentrated in the shell region behind the shock front and a negligible amount of particles occupies the central hot core. Local thermal equilibrium among the neutral atoms, instead of Saha equation, is assumed in this shell region. The absorptions calculated by considering the photoionization and the inverse bremsstrahlung of electrons in the field of neutral atoms in this shell region are not in very good agreement with the measured results. However, the agreement is always better than a factor of 10 and in fact better than a factor of 6 in all but one case. The discrepancies between the calculated and measured results may be attributed mainly to the use of the radius of the peak luminous volume, which is assumed to be spherical, as the actual shock radius.

In this thesis we have calculated the absorption coefficient per unit atom and electron due to the inverse bremsstrahlung of electrons in the field of neutron atoms as a function of the electron temperature and radiation frequency, and presented the results graphically. With these curves and the conventional formula for photoionization, one can now estimate the total absorption due to the photoionization and the inverse bremsstrahlung of electrons in the field of neutrals if the neutral density in the plasma is known.

The interpretation of the Litvak and Edwards absorption measurements in this thesis by considering only the above absorption mechanisms due to the neutral atoms and using the point explosion theory with certain plausible arguments to guess the electron density and temperature distributions is mainly suggestive. In the absence of any accurate information for the plasma size and of an explosion theory which takes into account the finite initial volume of the explosion, the agreement obtained in this work between the measured and calculated absorptions is considered as a strong evidence for the importance of neutral atoms in the interpretation of the absorption experiments in plasmas. In fact, the absorption due to the neutrals may even be the dominant heating mechanism which causes the explosion.

More experimental work designed primarily for the verification of the importance of the neutral atoms is needed.

APPENDIX A

DERIVATION OF EQUATION (II-42)

In Chapter II, we already obtained the following expressions

$$\sum_{n'\eta'\neq n\eta} \frac{|<n'\eta'|H^{I}|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} = \sum_{\substack{n'\neq n \\ \eta'\neq\eta}} \int_{-\infty}^{\infty} d\omega' \frac{|<n'\eta'|H^{PR1}|n\eta>|^2}{\hbar\omega'} \delta(\omega' - \frac{E_{n\eta}-E_{n'\eta'}}{\hbar}), \quad (A-1)$$

$$\sum_{n'\eta'\neq no} \frac{|<n'\eta'|H^{I}|no>|^2}{E_{no}-E_{n'\eta'}} = \sum_{\substack{n'\neq n \\ \eta'\neq o}} \int_{-\infty}^{\infty} d\omega' \frac{|<n'\eta'|H^{RR1}|no>|^2}{\hbar\omega'} \delta(\omega' - \frac{E_{no}-E_{n'\eta'}}{\hbar}). \quad (A-2)$$

The substitution of eq. (II-29) into the above expressions gives after using eqs. (II-23) and (II-30),

$$\sum_{n'\eta'\neq n\eta} \frac{|<n'\eta'|H^{I}|n\eta>|^2}{E_{n\eta}-E_{n'\eta'}} = \frac{1}{2\pi\hbar} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega' \frac{e^{i\omega' t'}}{\omega'}$$

$$\times \{ \sum_{n'\neq n} <n\eta|\underline{J}(\underline{r})\cdot \frac{\underline{\underline{A}}(\underline{r})}{c} |n'\eta+1><n'\eta+1|\underline{J}(\underline{r}'t')\cdot \frac{\underline{\underline{A}}(\underline{r}',\underline{t}')}{c} |n\eta>$$

$$+ \sum_{n'\neq n} <n\eta|\underline{J}(\underline{r})\cdot \frac{\underline{\underline{A}}(\underline{r})}{c} |n''\eta-1><n''\eta-1|\underline{J}(\underline{r}',t')\cdot \frac{\underline{\underline{A}}(\underline{r}',t')}{c} |n\eta> \} \quad (A-3)$$

$$\sum_{n'\eta'\neq no} \frac{|<n'\eta'|H^{I}|no>|^2}{E_{no}-E_{n'\eta'}} = \frac{1}{2\pi\hbar} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega' \frac{e^{i\omega' t'}}{\omega'}$$

$$\times \sum_{n'\neq n} <no|\underline{J}(\underline{r})\cdot \frac{\underline{\underline{A}}(\underline{r})}{c} |n'1_{\lambda k}><n'1_{\lambda k}|\underline{J}(\underline{r}'t')\cdot \frac{\underline{A}(\underline{r}',t')}{c} |no>. \quad (A-4)$$

Equation (A-4) and the first sum in the bracket of eq. (A-3) comes, respectively from letting $\eta'=1_{\lambda k}$ in eq. (A-2) and $\eta'=\eta+1$ in eq. (A-1). The second sum in the bracket of eq. (A-3) comes from letting $\eta'=\eta-1$ in eq. (A-1). Evaluating the matrix elements of $\underline{A}(\underline{r})$ and $\underline{A}(\underline{r},t)$ by eqs. (II-12) and (II-33) and assuming that the radiation field does not change appreciably over L^3, then

$$\sum_{n'\eta'\neq n\eta} \frac{|\langle n'\eta'|H^I|n\eta\rangle|^2}{E_{n\eta}-E_{n'\eta'}} - \sum_{n'\eta'\neq no} \frac{|\langle n'\eta'|H^I|no\rangle|^2}{E_{no}-E_{n'\eta'}}$$

$$= \sum_{\lambda k} \frac{\eta_\lambda(\underline{k})}{L^3\omega_k} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega' \Bigg\{ \frac{e^{i(\omega'+\omega_k)t'}}{\omega'}\, e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \sum_{n'\neq n}$$

$$\times \langle n|J_\lambda(\underline{r})|n'\rangle\langle n'|J_\lambda(\underline{r}'t')|n\rangle + \frac{e^{i(\omega'-\omega_k)t'}}{\omega'}\, e^{-i\underline{k}(\underline{r}-\underline{r}')} \sum_{n''\neq n}$$

$$\times \langle n|J_\lambda(\underline{r})|n''\rangle\langle n''|J_\lambda(\underline{r}',t')|n\rangle \Bigg\} \qquad \text{(A-5)}$$

where $J_\lambda(\underline{r},t) = \underline{J}(\underline{r},t)\cdot\underline{\epsilon}_\lambda(\underline{k})$. Let $\omega''=\omega'+\omega_k$ in the first term and $\omega''=-\omega'+\omega_k$ in the second term of eq. (A-5), then

$$\sum_{n'\eta'\neq n\eta} \frac{|\langle n'\eta'|H^I|n\eta\rangle|^2}{E_{n\eta}-E_{n'\eta'}} - \sum_{n'\eta'\neq no} \frac{|\langle n'\eta'|H^I|no\rangle|^2}{E_{no}-E_{n'\eta'}}$$

$$= \sum_{\lambda k} \frac{\eta_\lambda(\underline{k})}{L^3\omega_k} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega'' \Bigg\{ \frac{e^{i\omega''t'}}{\omega''-\omega_k}\, e^{i\underline{k}\cdot(\underline{r}-\underline{r}')} \sum_{n'\neq n} \langle n|J_\lambda(\underline{r})|n'\rangle\langle n'|J_\lambda(\underline{r}',t')|n\rangle$$

$$- \frac{e^{-i\omega''t'}}{\omega''-\omega_k}\, e^{-i\underline{k}\cdot(\underline{r}-\underline{r}')} \sum_{n''\neq n} \langle n|J_\lambda(\underline{r})|n''\rangle\langle n''|J_\lambda(\underline{r}',t')|n\rangle \Bigg\} \qquad \text{(A-6)}$$

Interchanging $(r,\underline{r}')$ and letting $t'=-t'$ in the second term of eq. (A-6), and summing the intermediate states $|n'\rangle$ and $|n''\rangle$, one finally obtains eq. (II-42)

$$\sum_{n'\eta'\neq n\eta} \frac{|\langle n'\eta'|H^I|n\eta\rangle|^2}{E_{n\eta}-E_{n'\eta'}} - \sum_{n'\eta'\neq no} \frac{|\langle n'\eta'|H^I|no\rangle|^2}{E_{no}-E_{n'\eta'}}$$

$$= - \sum_{\lambda k} \frac{\eta_\lambda(\underline{k})}{L^3\omega_k} \int d^3r \int d^3r' \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega' \frac{e^{i\omega' t'}}{\omega'-\omega_k} e^{i\underline{k}\cdot(\underline{r}-\underline{r}')}$$

$$\times \langle n|J_\lambda(\underline{r}')J_\lambda(\underline{r},-t')-J_\lambda(\underline{r})J_\lambda(\underline{r},t')|n\rangle \qquad \text{(II-42)}$$

APPENDIX B

SECOND QUANTIZATION

In this appendix, we shall express the potentials V^{Ae}, V^{ie}, V^{Ai} and the interactions V_A, V_e, and V_i in terms of the particle creation and destruction operators by second quantization. In section III-1, V^{Ae} represents the sum of the potentials between an electron and an atom, i.e.,

$$V^{Ae} = \sum_{\sigma m} V^{Ae}_{\sigma m}$$

where

$$V^{Ae}_{\sigma m} = - \frac{ze^2}{|\underline{R}_\sigma - \underline{r}_m|} + \sum_{j=1}^{z} \frac{e^2}{|\underline{R}_\sigma + \underline{\rho}_{\sigma j} - \underline{r}_m|}$$

is the potential between the σ-th atom and the m-th free electron with $\underline{r}_m$ and $\underline{R}_\sigma$ being the positions of the free electron and the nucleus. $\underline{\rho}_{\sigma j}$ is the position of the j-th atomic electron with respect to R_σ. In second quantization, V^{Ae} can be written as

$$V^{Ae} = \sum_{\substack{\underline{K}a \\ \underline{K}'a' \\ \underline{uu}'}} \langle \underline{K}'a'\underline{u}'| - \frac{ze^2}{|\underline{R}-\underline{r}|} + \sum_{j=1}^{z} \frac{e^2}{|\underline{R}+\underline{\rho}_j-\underline{r}|} |\underline{K}a\underline{u}\rangle A^\dagger(\underline{K}'a')A^\dagger(\underline{u}')A(\underline{K}a)A(\underline{u}) \qquad \text{(B-1)}$$

where $A(\underline{u})$ is the destruction operator of destructing a free electron of momentum $\hbar\underline{u}$ and $A(\underline{K}a)$ is that of destructing an atom of the external momentum $\hbar\underline{K}$ and the internal state $|a\rangle$. $A^\dagger(\underline{u}')$ and $A^\dagger(\underline{K}'a')$ are, respectively, the creation operators of creating a free electron of momentum $\hbar\underline{u}'$ and an atom of external momentum $\hbar\underline{K}'$ and the internal state $|a'\rangle$.

The wave function of a free electron is given by

$$|u\rangle = \frac{1}{L^{3/2}} e^{i\underline{u}\cdot\underline{r}} \qquad \text{(B-2)}$$

and the wave function of describing the external and internal states of an atom is given by

$$|\underline{K}a\rangle = \frac{1}{L^{3/2}} e^{i\underline{K}\cdot\underline{R}} |a\rangle \qquad \text{(B-3)}$$

where we have assumed that the center-of-mass coordinates of the atom coincide with its nucleus coordinates. Substituting eqs. (B-2) and (B-3) into eq. (B-1), one obtains

$$V^{Ae} = \sum_{\substack{\underline{K}a \\ \underline{K}'a' \\ \underline{u}\underline{u}'}} \frac{4\pi e^2 \delta_K(\underline{K}-\underline{K}'+\underline{u}-\underline{u}')}{L^3 |\underline{u}-\underline{u}'|^2} \langle a'|-z+\sum_{j=1}^{z} e^{i(\underline{u}-\underline{u}')\cdot\underline{\rho}_j}|a\rangle$$

$$\times A^\dagger(\underline{K}'a')A^\dagger(\underline{u}')A(\underline{K}a)A(\underline{u}) \qquad \text{(III-2)}$$

where the subscript K of δ_K denotes the Kronecker delta.

In the same way, one can obtain

$$V^{Ai} = \sum_{\substack{\underline{K}a\underline{K}'a' \\ \underline{\ell}b\underline{\ell}'b'}} \frac{4\pi e^2 \delta_K(\underline{K}-\underline{K}'+\underline{\ell}-\underline{\ell}')}{L^3 |\underline{K}-\underline{K}'|^2} \langle a'|z-\sum_{j=1}^{z} e^{-i(\underline{K}-\underline{K}')\cdot\underline{\rho}_j}|a\rangle$$

$$\times \langle b'|z-\sum_{j=1}^{z-1} e^{i(\underline{K}-\underline{K}')\underline{\rho}_j}|b\rangle A^\dagger(\underline{K}'a')A^\dagger(\underline{\ell}'b')A(\underline{K}a)A(\underline{\ell}b) \qquad \text{(III-3)}$$

$$V^{ie} = \sum_{\substack{\underline{\ell}b \\ \underline{\ell}'b \\ \underline{u}\underline{u}'}} \frac{4\pi e^2 \delta_K(\underline{\ell}-\underline{\ell}'+\underline{u}-\underline{u}')}{L^3 |\underline{u}-\underline{u}'|^2} \langle b'|-z+\sum_{j=1}^{z-1} e^{i(\underline{u}-\underline{u}')\cdot\underline{\rho}_j}|b\rangle$$

$$\boxtimes A^{\dagger}(\underline{\ell}'b')A^{\dagger}(\underline{u}')A(\underline{\ell}b)A(\underline{u}) \qquad \text{(III-4)}$$

where $A^{\dagger}(\underline{\ell}b)$ and $A(\underline{\ell}b)$ have the same meanings as $A^{\dagger}(\underline{K}'a')$ and $A(\underline{K}a)$.

In section III-1, V_A is the interaction of the atoms with radiation

$$V_A = -\sum_{\sigma j} \frac{e_{\sigma j}}{m_{\sigma j} c} \underline{p}_{\sigma j} \cdot \underline{A}(\underline{r}_{\sigma j}) = -\sum_{\sigma} \frac{ze}{m_{\sigma} c} \underline{p}_{\sigma} \cdot \underline{A}(\underline{r}_{\sigma}) + \sum_{\sigma j=1}^{z} \frac{e}{mc} \underline{p}_j \cdot \underline{A}(\underline{r}_{\sigma j})$$

where $\underline{A}(\underline{r})$ is given by (II-7). m_{σ} and m, $\underline{p}_{\sigma}$ and $\underline{p}_{\sigma j}$, and $\underline{r}_{\sigma}$ and $\underline{r}_{\sigma j}=\underline{r}_{\sigma}+\underline{\rho}_{\sigma j}$ are, respectively, the masses, the momenta, and the positions of the nucleus and the j-th atomic electron in the σ-th atom. Neglecting the first sum as compared to the second one because $m_{\sigma} \gg m$, V_A can be written, in second quantization, as

$$V_A = \sum_{\substack{\underline{K}a \\ \underline{K}'a'}} \langle \underline{K}'a'|\frac{e}{mc} \sum_{j=1}^{z} \underline{p}_j \cdot \underline{A}(\underline{r}_j)|\underline{K}a\rangle A^{\dagger}(\underline{K}'a')A(\underline{K}a).$$

Assuming that the center-of-mass coordinates of an atom coincide its nucleus coordinates, the substitution of eqs. (II-7) and (B-3) gives

$$V_A = \sum_{\substack{\lambda\underline{k} \\ \underline{K}a \\ \underline{K}'a'}} \frac{e}{mc} \sqrt{\frac{2\pi\hbar c^2}{L^3 \omega}}\, \delta_K(\underline{K}-\underline{K}'-\underline{k})\{\alpha_{\lambda}(\underline{k})\epsilon_{\lambda}(\underline{k})+\alpha_{\lambda}^{\dagger}(-\underline{k})\epsilon_{\lambda}(-\underline{k})\}\cdot\langle a'|\sum_{j=1}^{z} e^{-i\underline{k}\cdot\underline{\rho}_j}\underline{p}_j|a\rangle$$

$$\boxtimes A^{\dagger}(\underline{K}'a')A(\underline{K}a)$$

Using dipole moment approximation $e^{-i\underline{k}\cdot\underline{\rho}_j} \approx 1$, one obtains, after substituting

$$\underline{p}_j = \frac{i}{\hbar} m [H_A^{int}, \underline{\rho}_j]$$

where H_A^{int} is the hamiltonian of the internal motion of an atom,

$$V_A = \sum_{\substack{\lambda\underline{k} \\ \underline{K}a \\ \underline{K}'a'}} \frac{ie}{c} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}}\, \delta_K(\underline{K}-\underline{K}'-\underline{k})\omega_{a'a}\, \underline{d}_{a'a}\cdot[\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})]$$

$$\times A^\dagger(\underline{K}'a')A(\underline{K}a) \qquad \text{(III-5)}$$

where $\hbar\omega_{a'a} = E_{a'}-E_a$ is the energy difference between the internal states $|a'\rangle$ and $|a\rangle$ and $e\underline{d}_{a'a} = \langle a'| \sum_{j=1}^{z} e\underline{\rho}_j|a\rangle$ is the dipole moment transition of the atom from the state $|a\rangle$ to the state $|a'\rangle$.

In the same way, the interaction of the free electron with the radiation field

$$V_e = \sum_{j=1}^{Ne} \frac{e}{mc}\, \underline{p}_j\cdot\underline{A}(\underline{r}_j)$$

can be written, in second quantization, as

$$V_e = \sum_{\substack{\lambda\underline{k} \\ \underline{u}\underline{u}'}} \frac{e\hbar}{mc} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}}\, \{\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\}\cdot\underline{u}\; \delta_K(\underline{u}-\underline{u}'-\underline{k})\; A^\dagger(\underline{u}')A(\underline{u}) \qquad \text{(III-6)}$$

The interaction between the ions and the radiation is given, in second quantization, as

$$V_i = \sum_{\substack{\lambda\underline{k} \\ \underline{\ell}b \\ \underline{\ell}'b'}} \frac{ie}{c} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega}}\, \delta_K(\underline{\ell}-\underline{\ell}'-\underline{k})\omega_{b'b}\, \underline{d}_{b'b}\cdot\{\alpha_\lambda(\underline{k})\underline{\epsilon}_\lambda(\underline{k})+\alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\}A^\dagger(\underline{\ell}'b')A(\underline{\ell}b) \qquad \text{(III-7)}$$

where $\hbar\omega_{b'b} = E_{b'} - E_b$ and

$$\underline{d}_{b'b} = \langle b'| \sum_{j=1}^{z-1} \underline{\rho}_j |b\rangle .$$

APPENDIX C

NO PHOTONS EMITTED OR ABSORBED THROUGH THE INTERACTION OF FREELY-MOVING ELECTRONS WITH A RADIATION FIELD

In appendix B, we have obtained that the interaction of freely-moving electrons with a radiation field is given by

$$V_e = \sum_{\substack{\lambda \underline{k} \\ \underline{u}\underline{u}'}} \frac{e\hbar}{mc} \sqrt{\frac{2\pi\hbar c^2}{L^3 \omega}} \{\alpha_\lambda^\dagger(\underline{k})\underline{\epsilon}_\lambda(\underline{k}) + \alpha_\lambda(-\underline{k})\underline{\epsilon}_\lambda(-\underline{k})\}\cdot \underline{u}\ \delta_K(\underline{u}-\underline{u}'-\underline{k}) A_\lambda^\dagger(\underline{u}')A(\underline{u}).$$

Assume that the photons can be emitted through the interaction, the number of photons with momentum $\hbar\underline{k}$ and polarization λ emitted per unit time from L^3 will be, from section III-2,

$$n_\lambda(\underline{k}) = \sum_{\beta\beta'\eta} \frac{2\pi}{\hbar} D_{\beta\eta,\beta\eta} |\langle\beta'\eta + 1|V_e|\beta\eta\rangle|^2\ \delta(E_{\beta'\eta+1} - E_{\beta\eta}).$$

Let the initial and final states of the electrons and photons be

$$|\beta\eta\rangle = |\ldots n(\underline{u}),\ n(\underline{u}')\ldots\rangle\ |\ldots\eta_\lambda(\underline{k})\ldots\rangle$$

$$|\beta',\eta+1\rangle = |\ldots n(\underline{u})-1,\ n(\underline{u}') + 1\ldots\rangle|\ldots\eta_\lambda(\underline{k}) + 1\ldots\rangle,$$

then

$$n_\lambda(\underline{k}) = \sum_{\underline{u}\underline{u}'} \frac{(2\pi e)^2\hbar^2}{m^2\omega L^3} (\underline{u}\cdot\underline{\epsilon}_\lambda)^2 (f_\lambda(\underline{k})+1)\ N(\underline{u})\ \delta_K(\underline{u}-\underline{u}'-\underline{k})\ \delta(E_{\underline{u}'} - E_{\underline{u}} + \hbar\omega)$$

$$= \sum_{\underline{u}} \frac{(2\pi e^2)^2\hbar^2}{m^2\omega L^3} (\underline{u}\cdot\underline{\epsilon}_\lambda)^2 (f_\lambda(\underline{k})+1)\ N(\underline{u})\ \delta(E_{\underline{u}-\underline{k}} - E_{\underline{u}} + \hbar\omega)\ .$$

Since the energy conserved delta function is contained in the above expression, $n_\lambda(\underline{k})$ is not zero if

$$E_{\underline{u}-\underline{k}} - E_{\underline{u}} + \hbar\omega = 0$$

i.e.,

$$\cos\Theta = \frac{c}{v} + \frac{1}{2}\frac{k}{u} \qquad \text{(C-1)}$$

where Θ is the angle between $\underline{k}$ and $\underline{u}$ and v is the speed of the incident electron. Since $\frac{c}{v} \geq 1$ and k and u are positive, (C-1) cannot hold. Therefore no photons will be emitted through the interaction of freely-moving electrons with a radiation field. In the similar way, one can obtain that no photons will be absorbed through the interaction of freely-moving electrons with a radiation field.

APPENDIX D

DERIVATION OF EQS. (IV-31a) THROUGH (IV-31f)

For derivation of eqs. (IV-31a) through (IV-31f), the values of the following 3j symbols taken from the literature[32] are needed.

j_1	j_2	j_3	m_1	m_2	m_3	$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2$
1	0	1	0	0	0	* 1/3
2	0	2	0	0	0	1/5
2	1	1	0	0	0	2/15
2	2	2	0	0	0	* 2/35
3	1	2	0	0	0	* 3/35
4	2	2	0	0	0	2/35
0	1	1	0	1	-1	1/3
2	1	1	0	1	-1	1/30
0	2	2	0	1	-1	* 1/5
0	2	2	0	2	-2	1/5
2	2	2	0	1	-1	1/70
2	2	2	0	2	-2	2/35
4	2	2	0	1	-1	8/315
4	2	2	0	2	-2	1/630

when one needs the values of $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ other than its square, the negative square root of the number should be taken if it is preceded with the star symbol *. Since the sum of j_1 j_2 and j_3 for each row in the above table is even, each of the 3j symbols in the above is invariant in a permutation of any two columns.

For convenience, we rewrite here eqs. (IV-20), (IV-22), (IV-23), and (IV-26)

$$G(n,n,q) = n^2 - 2R_e \sum_{\ell m} \langle n\ell m|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle + \sum_{\substack{\ell m\\ \ell' m'}} |\langle n\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle|^2 \qquad \text{(IV-20)}$$

$$G(n,n',q) = \sum_{\substack{\ell m\\ \ell' m'}} |\langle n'\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle|^2$$

$$\text{(IV-26)}$$

$$= \sum_{\ell\ell' p} |R_{p,n\ell,n'\ell'}(q)|^2 (2p+1)(2\ell+1)(2\ell'+1)\begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix}^2$$

$$\langle n'\ell' m'|e^{i\underline{q}\cdot\underline{r}}|n\ell m\rangle = \sum_{p=|\ell-\ell'|}^{\ell+\ell'} Y_{p,\ell m,\ell' m'} R_{p,n\ell,n'\ell'}(q) \qquad \text{(IV-22)}$$

$$Y_{p,\ell m,\ell' m'} = i^{p+2m'}(2p+1)\sqrt{(2\ell+1)(2\ell'+1)}\begin{pmatrix} p & \ell & \ell' \\ o & m & -m' \end{pmatrix}\begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix} \qquad \text{(IV-23)}$$

where p takes the integers between $|\ell-\ell'|$ and $\ell+\ell'$ such that $p+\ell+\ell'$ = even, otherwise $\begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix}$ vanishes.

For n'=n=1, it is easily to obtain that

$$G(1,1,q) = \{1-R_{0,10,10}(q)\}^2 \qquad \text{(IV-31a)}$$

For n'≠n, one obtains from eq. (IV-26) that

$$G(1,2,q) = \sum_{\ell' p} R^2_{p,10,2\ell'}(q)(2p+1)(2\ell'+1)\begin{pmatrix} p & o & \ell' \\ o & o & o \end{pmatrix}^2$$

$$= R^2_{0,10,20}(q) + 3R^2_{1,10,21}(q) \qquad \text{(IV-31b)}$$

$$G(1,3,q) = \sum_{\ell' p} R^2_{p,10,3\ell'}(q)(2p+1)(2\ell'+1)\begin{pmatrix} p & o & \ell' \\ o & o & o \end{pmatrix}^2$$

$$= R^2_{0,10,30}(q) + 3R^2_{1,10,31}(q) + 5R^2_{2,10,32}(q) \qquad \text{(IV-31c)}$$

$$G(2,3,q) = \sum_{\ell' p} R^2_{p,20,3\ell'}(q)(2p+1)(2\ell'+1)\begin{pmatrix} p & o & \ell' \\ o & o & o \end{pmatrix}^2$$

$$+ \sum_{\ell' p} 3R^2_{p,21,3\ell'}(q)(2p+1)(2\ell'+1)\begin{pmatrix} p & 1 & \ell' \\ o & o & o \end{pmatrix}^2$$

$$= R^2_{0,20,30}(q) + 3R^2_{1,20,31}(q) + 5R^2_{2,20,32}(q)$$

$$+ 3R^2_{1,21,30}(q) + 3R^2_{0,21,31}(q) + 6R^2_{2,21,31}(q)$$

$$+ 6R^2_{1,21,32}(q) + 9R^2_{3,21,32}(q) \qquad \text{(IV-31e)}$$

For n'=n=2,3, one obtains from eqs. (IV-20) and (IV-26) that

$$G(2,2,q) = 4-2\mathrm{Re}\{\langle 200|e^{i\underline{q}\cdot\underline{r}}|200\rangle + \langle 210|e^{i\underline{q}\cdot\underline{r}}|210\rangle + 2\langle 211|e^{i\underline{q}\cdot\underline{r}}|211\rangle\}$$

$$+ \sum_{\ell\ell' p} |R_{p,2\ell,2\ell'}(q)|^2(2p+1)(2\ell+1)(2\ell'+1)\begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix}^2$$

$$G(3,3,q) = 9-2\mathrm{Re}\{\langle 300|e^{i\underline{q}\cdot\underline{r}}|300\rangle + \langle 310|e^{i\underline{q}\cdot\underline{r}}|310\rangle + \langle 320|e^{i\underline{q}\cdot\underline{r}}|320\rangle$$

$$+ 2\langle 311|e^{i\underline{q}\cdot\underline{r}}|311\rangle + 2\langle 321|e^{i\underline{q}\cdot\underline{r}}|321\rangle + 2\langle 322|e^{i\underline{q}\cdot\underline{r}}|322\rangle\}$$

$$+ \sum_{\ell\ell p} |R_{p,3\ell,3\ell'}(q)|^2(2p+1)(2\ell+1)(2\ell'+1)\begin{pmatrix} p & \ell & \ell' \\ o & o & o \end{pmatrix}^2$$

The terms in the brackets of the above two equations are computed through the use of eqs. (IV-22) and (IV-23). Then

$$G(2,2,q) = 4-2\{R_{0,20,20}(q) + 2R_{0,21,21}(q) + 2R_{2,21,21}(q) + R_{0,21,21}(q)-2R_{2,21,21}(q)\}$$

$$+ \sum_{\ell' p} R^2_{p,20,2\ell'}(q)(2p+1)(2\ell'+1) \begin{pmatrix} p & o & \ell' \\ o & o & o \end{pmatrix}^2$$

$$+ \sum_{\ell' p} 3R^2_{p,21,2\ell'}(q)(2p+1)(2\ell'+1) \begin{pmatrix} p & 1 & \ell' \\ o & o & o \end{pmatrix}^2$$

$$= 4-2R_{0,20,20}(q) + R^2_{0,20,20}(q) - 6R_{0,21,21}(q) + 3R^2_{0,21,21}(q)$$

$$+ 6R^2_{1,20,21}(q) + 6R^2_{2,21,21}(q) \qquad \text{(IV-31d)}$$

$$G(3,3,q) = 9-2\{R_{0,30,30}(q) + 3R_{0,31,31}(q) + 5R_{0,32,32}(q)\}$$

$$+ \sum_{\ell' p} R^2_{p,30,3\ell'}(q)(2p+1)(2\ell'+1) \begin{pmatrix} p & o & \ell' \\ o & o & o \end{pmatrix}^2$$

$$+ \sum_{\ell' p} 3R^2_{p,31,3\ell'}(q)(2p+1)(2\ell'+1) \begin{pmatrix} p & 1 & \ell' \\ o & o & o \end{pmatrix}^2$$

$$+ \sum_{\ell' p} 5R^2_{p,32,3\ell'}(q)(2p+1)(2\ell'+1) \begin{pmatrix} p & 2 & \ell' \\ o & o & o \end{pmatrix}^2$$

$$= 9-2R_{0,30,30}(q) + R^2_{0,30,30}(q) - 6R_{0,31,31}(q) + 3R^2_{0,31,31}(q)$$

$$- 10R_{0,32,32}(q) + 5R^2_{0,32,32}(q) + 6R^2_{1,30,31}(q) + 12R^2_{1,31,32}(q)$$

$$+ 6R^2_{2,31,31}(q) + \frac{50}{7} R^2_{2,32,32}(q) + 10R^2_{2,30,32}(q) + 18R^2_{3,31,32}(q)$$

$$+ \frac{90}{7} R^2_{4,32,32}(q). \qquad \text{(IV-31f)}$$

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