Lower bound on the Rosseland mean free path

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Starting with an oscillator-strength sum rule, we derive an integral relation which must be satisfied by the bound-electron radiation absorption coefficient in a plasma, when the distribution of ions with respect to degree of ionization and excitation state is arbitrary. Making use of this relation, we formulate and solve a variational problem which, under conditions of local thermodynamic equilibrium, yields the smallest possible value of the Rosseland mean free path l_R. We compare the estimated minimum l_R with estimates of the actual value of this quantity in the presence of multiply charged ions, using a lead plasma as an example.

1. INTRODUCTION

The correct treatment of radiative transfer in a plasma is of the greatest importance in the hydrodynamics of high-temperature phenomena.[1] The simplest case, that of a plasma transparent to its own radiation, reduces to a consideration of bulk radiative energy losses. In a fully ionized plasma, these are the well known bremsstrahlung losses. In an incompletely ionized plasma of multiply charged heavy ions, calculations of bulk energy losses must incorporate free-bound (recombination radiation) and bound-bound (line) transitions as well as free-free transitions. The situation is considerably more complicated when the plasma becomes optically thick. Quantitative analysis is especially difficult in the intermediate case of a plasma which is optically thick in some parts of the spectrum (in particular, in the lines of bound-bound transitions) while remaining transparent in others. Clearly, the hydrodynamic problem must then be solved in conjunction with the radiative transfer equations, which include the effects of plasma opacity. It could be said that an increase in plasma density gives rise to an increase in opacity, although the accurate criterion is actually that the photon mean free path (in some region of the spectrum) becomes less than some characteristic linear dimension of the plasma. This also often occurs in a plasma with multiply charged heavy ions, in which the photon absorption cross sections are particularly large in certain regions of the spectrum which are generally narrow, and which correspond to the discrete spectral lines of these ions.

One field which has aroused great interest is the hydrodynamics of high-temperature phenomena associated with inertially confined thermonuclear fusion, where the compression of thermonuclear targets to extremely high densities plays a pivotal role (see the collections of articles, for example, in Refs. 2 and 3). Under the physical conditions needed to initiate thermonuclear fusion, the plasma density in the target shell must be hundreds of times higher than the density of the solid material, with a temperature measured in thousands of electron volts ($\sim 10^7$ K)—the characteristic temperature for ignition of a thermonuclear reaction at the center of the target, which contains hydrogen fuel. Consequently, we need to know the physical properties of an inhomogeneous dense plasma, which in general is not an ideal gas, particularly the mean free path of radiation within it as a function of frequency.

In practice, such a plasma exists in a state of local thermodynamic equilibrium (LTE) between the matter and the internal radiation. Radiative transfer may then be treated in a radiative thermal conductivity approximation, which follows directly from the radiative transfer equations in the limit of a plasma which is optically thick over the entire spectrum. This approximation is applicable when the photon mean free path, as a function of frequency, is less than some characteristic hydrodynamic dimension of the inhomogeneous moving plasma (this dimension is obviously always less than the linear size of the plasma, as was mentioned previously). The radiative thermal conductivity approximation is widely known, and has been discussed in connection with many problems in physics[1] and astrophysics.[4] To implement it, one need know only the Rosseland mean free path of the photons. In general, the Rosseland mean free path is obtained by integrating the reciprocal of the absorption coefficient over frequency, i.e., the photon mean free path with the Rosseland weighting function, which is proportional to the partial derivative with respect to temperature of the equilibrium Planck function. This makes it clear that bound-bound transitions can make a significant contribution to the Rosseland mean free path only when some mechanism broadens the corresponding absorption lines sufficiently. For the natural linewidths, which are in fact small, this contribution can usually be neglected.[1]

Thus, in order to compute the radiative transfer of energy in an inhomogeneous plasma, it is necessary to know the spectral dependence of the photon absorption coefficient. In a plasma consisting of multiply charged heavy ions, the most difficult aspect is taking bound-bound transitions into account,[1] since in order to do so, one needs to be concerned with the distribution of ions in various ionization levels, take an enormous number of transitions between a multitude of quantum states of complex ions into consideration, and calculate spectral line broadening due to all possible mechanisms. In a dense, nonideal plasma, this task is even further complicated by the fact that strictly speaking, one needs to calculate the structure of the quantum levels not of a single

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isolated ion, but of a whole group of interacting ions and electrons in a state of thermal agitation.

The contributions of bound-bound transitions, i.e., line absorption effects, have been discussed in a great deal of detail in the review by Cox.[5] It was emphasized there for the first that taking bound-bound transitions into consideration can result in a marked (severalfold) reduction in the Rosseland mean free path, as, for example, under considerations indicated previously for inertially confined thermonuclear fusion.

If the mean level of ionization of the plasma is known, we can obviously make fairly accurate allowances for the contributions of bremsstrahlung and scattering from free electrons; however, as we have already pointed out, we have practically no detailed information on the role of bound-bound transitions, and only extremely sketchy data on free-bound transitions (with regard to the latter, for example, see Ref. 1). Under these circumstances, it is natural to reformulate the calculation of the Rosseland mean free path in such a way that for given frequency-dependent absorption and free-electron scattering coefficients, we take the contribution of all transitions from bound states (both bound-bound-and bound-free) to be an unknown function of frequency, which must satisfy some general requirements. For the general requirement on the absorption coefficient, we make use of an oscillator-strength sum rule derived for dipole transitions of an arbitrary atomic system in the field of a light wave.[6] As we show below, this approach can be rigorously followed within the scope of the classical Euler-Lagrange variational problem, the Rosseland mean free path itself playing the role of the functional being varied. In other words, having solved the variational problem, we will obtain, for any given plasma temperature T and density ρ, a lower bound on the Rosseland mean free path (it is generally clear from physical considerations that the extremum is a minimum in the present case). We will demonstrate below that in a dense plasma, this estimate of the minimum is quite close (within a factor of 2 or 3) to the actual value.

In the present paper, when we calculate the lower bound, we assume for simplicity that we have a plasma in statistical equilibrium containing ions of only a single element, with atomic number Z and atomic weight A. The generalization to a mixture of different elements is not at all difficult, since in the ultimate formulas only the mean density of bound electrons appear. In a low-density plasma, this comes from the Saha equation, while in a dense plasma, it can be estimated in a mean-ion approximation.[7]

Furthermore, we shall completely neglect collective effects in the propagation of electromagnetic waves in plasma; that is, we assume $\hbar\omega_p \ll T$ (where ω_p is the plasma frequency). Finally, we emphasize that this work does not pretend to derive strictly accurate quantitative results for the Rosseland mean free path over a wide range of temperature and density in any material. Nevertheless, the method we propose and the simple formulas derived make it possible, in every specific instance, to obtain an estimate of the minimum Rosseland mean free path which is close to the actual value over a certain range of parameters.

2. ROSSELAND MEAN FREE PATH AND AN OSCILLATOR-STRENGTH SUM RULE

In the situation we are considering, the Rosseland mean free path l_R is defined by[4]

$$l_R=\int_0^\infty \frac{R(u)}{k_{be}^*(\nu)+k_{fe}^*(\nu)+k_s}\,du, \tag{1}$$

$$R(u)=(15/4\pi^4)u^4e^{-u}(1-e^{-u})^{-2} \tag{2}$$

is the Rosseland function; $u = h\nu/T$ is a dimensionless frequency; $k_{be}{}^*(\nu)$ and $k_{fe}{}^*(\nu)$ (measured in cm^{-1}) are the bound- and free-electron radiation absorption coefficients, respectively (the asterisks denote the fact that they must be corrected for induced emission)$^{(1)}$; k_s (cm^{-1}) is the free-electron scattering coefficient (which is frequency-independent in the Thomson scattering approximation, and requires no correction for induced scattering). In accordance with these definitions, we assume that $k_{fe}{}^*(\nu)$ is a known function of frequency and k_s is a known constant, while $k_{be}{}^*(\nu)$ is an unknown function which satisfies

$$\int_0^\infty k_{be}^*(\nu)\,d\nu=\frac{\pi e^2}{m_e c}N_{be}, \tag{3}$$

and which must be determined by finding an extremum of the functional (1). We now demonstrate how condition (3) follows from a theorem on the sum of oscillator strengths (the Thomas-Reiche-Kuhn sum rule[8]).

We consider an atom (ionized i times) which contains $Z - i$ bound electrons, and which lies in quantum state n with excitation energy ε_n^i (by n, we mean the entire set of quantum numbers specifying the state of the atom; the excitation energy is measured from the ground state). In general, the absorption of electromagnetic radiation is accompanied by the following types of transitions in the overall system of atoms and free electrons: bound-bound transitions $n \to n'$, bound-free $n \to c$ and free-bound $c \to n$ transitions, as well as free-free transitions $c \to c'$. We make use of the Thomas-Reiche-Kunh sum rule for those transitions, and only those, for which the initial states are discrete states. In other words, we assume that the unknown term $k_{be}{}^*(\nu)$ derives from the collective contribution of all transitions of the types $n \to n'$ and $n \to c$, while the remaining $c \to n$ and $c \to c'$ transitions are included in the known term $k_{fe}{}^*(\nu)$.

In the general case, $n \to n'$ transitions can occur both with absorption of a photon of frequency

$$\nu_{nn'}^i=(\varepsilon_{n'}{}^i-\varepsilon_n{}^i)/h \tag{4}$$

(true absorption, $\nu_{nn'}^i > 0$) and with emission of a photon of frequency $-\nu_{nn'}^i$ (induced emission, $\nu_{nn'}^i < 0$). Transitions at positive frequencies $\nu_{nn'}^i$ give a positive contribution to the absorption coefficient $k_{be}{}^*$, and those at negative frequencies give a negative contribution. The latter statement is also true for $n \to c$ transitions (excitation energy $\varepsilon_{n'}^i$ is simply replaced by ε_c^i). As a result, the total absorption coefficient $k_{be}{}^*$ is an algebraic sum of positive and negative absorption terms, which correspond to the positive and negative frequencies of the appropriate transitions.

The oscillator strength $f^{i}_{nn'}$ of a dipole transition $n \to n'$ is defined[8,1] in such a way that

$$\int \sigma^{i}_{nn'}(\nu)\,d\nu = \frac{\pi e^2}{m_e c} f^{i}_{nn'}, \tag{5}$$

where $\sigma^{i}_{nn'}(\nu)$ is the absorption cross section for electromagnetic radiation, having the form of a narrow resonance near the transition frequency $\nu^{i}_{nn'}$ (negative values of $f^{i}_{nn'}$ and $\sigma^{i}_{nn'}$ correspond to negative frequencies $\nu^{i}_{nn'}$). For transitions $n \to c$, the concept of a differential oscillator strength is usually employed[8,1], being defined by

$$(df/d\nu)_{nc}{}^{i} = (m_e c/\pi e^2)\,\sigma_{nc}{}^{i}(\nu), \tag{6}$$

where $\sigma^{i}_{nc}(\nu)$ is the photoionization cross section of an i-times ionized atom in state n, which is non-zero for frequencies $\nu > \nu^{i}_{nc,th}$, where $\nu^{i}_{nc,th}$ is the photoionization threshold. With this notation, the Thomas-Reiche-Kuhn sum rule is of the form[8]

$$\sum_{n'} f^{i}_{nn'} + \int\limits_{\nu^{i}_{nc,th}}^{\infty} \left(\frac{df}{d\nu}\right)^{i}_{nc} d\nu = Z - i. \tag{7}$$

For subsequent developments, it will be convenient to introduce a total absorption cross section $\sigma^{i}_{n}(\nu)$ for an i-times ionized atom in state n, determined by the entire set of transitions $n \to n'$ and $n \to c$. In the limit of infinitely narrow bound-bound transitions, according to (5) and (6), we have

$$\sigma_n{}^{i}(\nu) = \sum_{n'} \sigma^{i}_{nn'}(\nu) + \sigma_{nc}{}^{i}(\nu) = \frac{\pi e^2}{m_e c} \sum_{n'} f^{i}_{nn'}\,\delta(\nu - \nu^{i}_{nn'})$$

$$+ \frac{\pi e^2}{m_e c} \begin{cases} 0, & \nu < \nu^{i}_{nc,th} \\ (df/d\nu)_{nc}{}^{i}, & \nu \geqslant \nu^{i}_{nc,th} \end{cases}. \tag{8}$$

It follows from the discussion above that the frequency ν in (8) can take on any value in the range $-\varepsilon^{i}_{n}/h \leqslant \nu < \infty$, with $\sigma^{i}_{n}(\nu) > 0$ for $\nu > 0$ and $\sigma^{i}_{n}(\nu) < 0$ for $\nu < 0$. With the definition (8), the sum rule (7) takes the form

$$\int\limits_{-\varepsilon_n{}^{i}/h}^{+\infty} \sigma_n{}^{i}(\nu)\,d\nu = \frac{\pi e^2}{m_e c}(Z - i). \tag{9}$$

The total absorption coefficient $k_{be}{}^{*}(\nu)$ for bound electrons makes physical sense only for positive frequencies, and may be expressed in terms of $\sigma^{i}_{n}(\nu)$ in the following manner:

$$k_{be}{}^{*}(\nu) = \sum_{i,n} N_n{}^{i}\left[\sigma_n{}^{i}(\nu) + \begin{cases} 0, & \varepsilon_n{}^{i}/h < \nu \\ \sigma_n{}^{i}(-\nu), & 0 \leqslant \nu \leqslant \varepsilon_n{}^{i}/h \end{cases}\right]. \tag{10}$$

Here N^{i}_{n} (cm^{-3}) is the number of i-times ionized atoms in state n per unit volume. Bearing in mind that

$$N_{be} = \sum_{i} (Z - i) \sum_{n} N_n{}^{i}, \tag{11}$$

we obtain (3) directly from (9) and (10). We emphasize that Eq. (10) and the integral relation (3) hold for arbitrary (and not just equilibrium) distributions of ions in the various excitation and ionization states.

If the bound-bound transitions are not taken to be infinitely narrow, but instead we incorporate the actual (i.e., broadened) spectral line profiles, then these profiles must be substituted into (8) instead of δ-functions. Accordingly, we must give up the exact photoionization threshold $\nu^{i}_{nc,th}$, formally replacing this quantity by zero. Furthermore, in Eqs. (9) and (10), instead of the exact value ε^{i}_{n}/h of the frequency, we need an infinite quantity which allows for an arbitrarily broadened given state and ground state. It is easy to see that these changes have no effect on the derivation of Eq. (3).

The definition of the absorption coefficient (10) assumed in the present paper, which is corrected for induced emission, differs somewhat from the conventional definition. However, if from $k_{be}{}^{*}$ we omit the term $k_{bb}{}^{*}$, due solely to bound-bound transitions [first term on the right-hand side of (8)], we obtain from (8) and (10)

$$\int\limits_{0}^{\infty} k_{bb}{}^{*}(\nu)\,d\nu = \frac{\pi e^2}{m_e c} \sum_{i,n,n'} N_n{}^{i} f^{i}_{nn'} = \frac{\pi e^2}{m_e c} \sum_{i,n,n'>n} (N_n{}^{i} f^{i}_{nn'} + N_{n'}{}^{i} f^{i}_{n'n})$$

$$= \frac{1}{c} \sum_{i,n,n'>n} |h\nu^{i}_{nn'}|\,(N_n{}^{i} B^{i}_{nn'} - N_{n'}{}^{i} B^{i}_{n'n}). \tag{12}$$

In order to go from a full sum over n' above to a sum over $n' > n$, for "positive transitions" with $\nu^{i}_{nn'} > 0$, in the double sum

$$\sum_{n,n'>n} N_n{}^{i} f^{i}_{nn}$$

we have changed the order of summation,

$$\sum_{n',n>n'} N_n{}^{i} f^{i}_{nn'}$$

and interchanged the summation indices n and n':

$$\sum_{n,n'>n} N_{n'}{}^{i} f^{i}_{n'n}.$$

We have taken the usual definitions[9,10] of the Einstein coefficients $B^{i}_{nn'}$ and $B^{i}_{n'n}$. In the LTE approximation, where the excited states are populated in accordance with Boltzmann statistics and $N^{i}_{n} \sim g^{i}_{n} \exp(-\varepsilon^{i}_{n}/T)$, the relation[10]

$$g_{n'}{}^{i} f^{i}_{n'n} = -g_n{}^{i} f^{i}_{nn'} \tag{13}$$

enables us to transform (12) to the well known form[4]

$$\int\limits_{0}^{\infty} k_{bb}{}^{*}(\nu)\,d\nu = \frac{\pi e^2}{m_e c} \sum_{i,n,n'>n} N_n{}^{i} f^{i}_{nn'} \left[1 - \exp\left(-\frac{h\nu^{i}_{nn'}}{T}\right)\right]. \tag{14}$$

Note that in the present case, the total absorption coefficient from bound states $k_{be}{}^{*}(\nu)$ cannot be transformed to the form (14), as $c \to n$ transitions (the inverse of $n \to c$ transitions) are included in the term $k_{fe}{}^{*}(\nu)$.

3. SOLUTION OF THE VARIATIONAL PROBLEM AND ESTIMATION OF THE MINIMUM ROSSELAND MEAN FREE PATH

We are thus obliged to find an extremum of the function (1) with the constraint (3). We introduce the notation

$$\varphi(u)=k_{be}^*(\nu),\quad F(u)=k_{fe}^*(\nu)+k_s, \tag{15}$$

$$\int_0^\infty \varphi(u)\,du=k_0=\frac{\pi e^2}{m_e c}\frac{h}{T}N_{be} \tag{16}$$

and consider first the simpler case $F(u)=0$. To solve the variational problem, we employ Lagrange's method of undetermined multipliers,[11] i.e., we seek an unconditional extremum of the functional

$$L(\varphi,\lambda)=\int_0^\infty \frac{R}{\varphi}du+\lambda\Big(\int_0^\infty \varphi\,du-k_0\Big). \tag{17}$$

Equating the variational derivative $\partial L/\partial\varphi$ to zero, we obtain

$$\varphi(u)=\lambda^{-1/2}R^{1/2}(u). \tag{18}$$

Substituting (18) into the auxiliary equation (3), we find the values of λ, φ, and $l_{R,\min}$:

$$\lambda=\Big(\int_0^\infty R^{1/2}du\Big)^2 k_0^{-2}=\frac{735}{\pi^4}\zeta^2(3)k_0^{-2}, \tag{19}$$

$$\varphi(u)\equiv k_{be}^*(\nu)=\Big(\int_0^\infty R^{1/2}du\Big)^{-1}k_0R^{1/2}(u)$$

$$=\frac{k_0}{14\zeta(3)}u^2e^{-u/2}(1-e^{-u})^{-1}, \tag{20}$$

$$l_{R,\min}[\mathrm{cm}]=\Big(\int_0^\infty R^{1/2}du\Big)^2 k_0^{-1}=\frac{735}{\pi^4}\zeta^2(3)k_0^{-1}$$

$$=1{,}65\cdot10^{-4}\frac{A}{Z-\bar{i}}\frac{T[\mathrm{keV}]}{\rho[\mathrm{g\cdot cm^{-3}}]}. \tag{21}$$

Here $\xi(x)$ is the Riemann zeta function, and $\bar{i}$ is the mean ionization level. It can be shown by direct substitution that (19)–(21) do in fact minimize the functional (1).

Carrying out a similar computation for $F(u)\neq0$, we obtain

$$\varphi(u)=\Big(k_0+\int_0^\infty F\,du\Big)\Big(\int_0^\infty R^{1/2}du\Big)^{-1}R^{1/2}(u)-F(u). \tag{22}$$

However, from a practical standpoint, this result is meaningless, as in a typical situation the integral of F will diverge at both limits of integration. Eliminating the divergence of this integral by artificially cutting it off, we obtain the absorption coefficient $k_{be}^*(\nu)\equiv\varphi(u)$, which may be positive or negative. This leads to the conclusion that when $F(u)\neq0$, the variational problem must be stated differently.

In general, the absorption coefficient $k_{be}^*(\nu)$ can take on negative values over some region of the spectrum (as happens in lasers, for instance). It is known that in LTE in a plasma of hydrogen-like ions, $k_{be}^*(\nu)>0$ for all $0<\nu<\infty$; the latter limit is likely to hold for plasmas of more complex ions as well. Similarly, the known term $k_{fe}^*(\nu)$ can in general be of either sign. However, when free-electron absorption or scattering must be taken into account under LTE conditions, $F(u)>0$ for all $0<\nu<\infty$. With an LTE orientation, we formulate the generalized variational problem (17) for the case $F(u)>0$, $\varphi(u)\geqslant0$. In more realistic complex situations, it is necessary to incorporate additional physical assumptions, allowing for an appropriate restriction or expansion of the class of functions $\varphi(u)$ for which one seeks an extremum of the functional (1).

When $F(u)>0$, the search for an extremum of (1) must be broadened to the class of functions of the form

$$\varphi(u)=\begin{cases}0, & 0\leqslant u\leqslant u_1,\\ \varphi(u)>0, & u_1<u<u_2,\\ 0, & u_2\leqslant u<\infty.\end{cases} \tag{23}$$

In other words, we must find an extremum of the functional

$$L(\varphi,u_1,u_2)=\int_0^{u_1}\frac{R}{F}du+\int_{u_1}^{u_2}\frac{R}{\varphi+F}du+\int_{u_2}^{\infty}\frac{R}{F}du \tag{24}$$

with the joining condition

$$\int_{u_1}^{u_2}\varphi\,du=k_0, \tag{25}$$

when the limits u_1 and u_2 are free parameters to be determined in the process of solving the variational problem. Methodologically, the search for an extremum of (24) does not differ from the case considered previously: to the condition for an extremum employed earlier, $\partial L/\partial\varphi=0$, we now add the conditions for an extremum within the finite range $u_1<u<u_2$ relative to the parameters u_1 and u_2, $\partial L/\partial u_1=\partial L/\partial u_2=0$, the expansion of which gives the following equations for u_1 and u_2:

$$\frac{R^{1/2}(u_1)}{F(u_1)}=\frac{R^{1/2}(u_2)}{F(u_2)}=\int_{u_1}^{u_2}R^{1/2}du\Big/\Big(k_0+\int_{u_1}^{u_2}F\,du\Big). \tag{26}$$

It can be proven that for functions $F(u)$ which behave in ways which are of physical interest, Eq. (26) has a unique solution with $u_1<u_2$. The lower bound on the Rosseland mean free path is then given [compared with (21)] by

$$l_{R,\min}=\int_0^{u_1}\frac{R}{F}du+\Big(\int_{u_1}^{u_2}R^{1/2}du\Big)^2\Big(k_0+\int_{u_1}^{u_2}F\,du\Big)^{-1}+\int_{u_2}^{\infty}\frac{R}{F}du. \tag{27}$$

To illustrate the quantitative difference between the variational problems (24) and (17), we consider an example with $k_s=k_0$, $k_{fe}^*(\nu)=0$. In that case, we find from (26) and (27) that $u_1=1.91$, $u_2=6.48$, $l_{R,\min}=0.867k_0^{-1}$ (when $k_s=0$, Eq. (21) gives $l_{R,\min}=10.9k_0^{-1}$). However, by simply substituting the solution (20) for $k_{be}^*(\nu)$ (which was obtained by assuming $k_s=k_{fe}^*=0$) along with $k_s=k_0$ into (1), we obtain almost exactly the same result: $l'_{R,\min}=0.904k_0^{-1}$.

Note that a decrease in $l_{R,\min}$ and $l'_{R,\min}$, which are practically equal, has no special physical meaning from the standpoint of a real free-electron scattering contribution to the Rosseland mean free path. In fact, the quantity k_s, which corresponds to Thomson scattering, will be $k_s=\sigma_T\bar{i}\rho/m_pA$, where $\sigma_T=0.67\cdot10^{-24}\ \mathrm{cm}^2$. It should be completely obvious that $k_0\gg k_s$ so long as $Z-\bar{i}\gtrsim1$, since from the definition of k_0 in (16), we have

$$\frac{\pi e^2 h}{m_e cT} N_{be} = \frac{\pi e^2 h}{m_c cT} (Z-\bar{i}) \frac{\rho}{Am_p} \gg \sigma_T \bar{i} \frac{\rho}{Am_p},$$

which, after substituting for all known constants, reduces to

$$T \ll 1{,}9 \cdot 10^{12} \mathrm{K} (Z-\bar{i})/\bar{i}.$$

The more free electrons there are, i.e., the closer the mean ionization level $\bar{i}$ is to Z (complete ionization of the atoms), the harder it is to satisfy this last condition. Nevertheless, with just the K-shell electrons remaining, the derived condition is satisfied for heavy atoms. Let us take $Z = 82$ and $\bar{i} = 80$ (lead with the K-shell electrons), so that we have an upper limit on the temperature: $T \ll 4.8 \cdot 10^{10}$ K. But even at $T \sim 5 \cdot 10^9$ K and densities which are not significantly different from normal, lead is quite deficient in K-shell electrons.

Without resorting to any new examples, it can be shown that the actual contribution of free-electron absorption or scattering to the desired quantity, $l_{R,\min}$, is generally extremely small. For practical estimates of the lower bound on the Rosseland mean free path in a plasma of multiply-charged heavy ions, we may therefore use the simple formula (21), which was derived using the first version of the variational problem. In the next section, we consider an important problem, concerning how close this lower bound is to the actual Rosseland mean free path.

4. COMPARISON OF THE LOWER BOUND AND ACTUAL VALUES OF THE ROSSELAND MEAN FREE PATH

When $I_i/T \gg 1$ in a low-density plasma, where I_i is the ionization potential of the ground state of an i-times ionized atom, we may use Eq. (12) of Ref. 12 for a realistic estimate of the quantity l_R; in our present notation, this is

$$l_{R,rp}[\mathrm{cm}] = 2.0 \cdot 10^{-3} (AT^2[\mathrm{keV}]/\rho[\mathrm{g \cdot cm^{-3}}]) (i+1)^{-2} \exp(I_i/T). \tag{28}$$

The hydrogen-like approximation and the exchange of summation over quantum states and integration used to derive (28) in Ref. 12 are inapplicable when the ground-state photoionization threshold $h\nu = I_i$ lies in the vicinity of the maximum of the Rosseland function (2). Since the function $R(u)$ attains its maximum at $u_m = 3.83$ and has a width at half-maximum of $\Delta u_{1/2} = 4.97$, the conditional limit of applicability of (28) can be taken to be $I_i/T > 5$.

In a dense plasma, where

$$I_i/T \leqslant 5 \tag{29}$$

and the main contribution to l_R comes from transitions out of the ground state, the actual value of l_R can be approximated in the following way. Rejecting the classical formula for absorption in lines due to bound electrons,[13] and assuming that for high frequencies, the quantum mechanical calculation (using Kramers' expression) gives $\sigma_1^i(\nu) \sim (\nu)^{-3}$, we approximate the ground-state absorption cross section by

$$\sigma_1{}^i(\nu) = \alpha a_0{}^2 \left(\frac{2I_\mathrm{H}}{I_i}\right)^3 \frac{a_i(h\nu/I_i)}{(h\nu/I_i)^4 + b_i(h\nu/I_i)^2 + c_i}, \tag{30}$$

where

$$\alpha = e^2/\hbar c, \qquad a_0 = \hbar^2/m_e e^2, \qquad 2I_\mathrm{H} = e^2/a_0.$$

To determine the three dimensionless constants a_i, b_i, and c_i in the supplement to the sum rule (9), we impose the following two conditions on $\sigma_1^i(\nu)$, which reflect the actual regularities in the behavior of that quantity: 1) the maximum cross section $\sigma_1^i(\nu)$ must occur for $h\nu = I_i$; 2) in the limit $h\nu \gg I_H Z^2$, Eq. (30) must go over into the Kramers expression for the K-shell photoeffect. In particular, for heavy elements ($Z \gg 1$) with $Z - i > 2$, we have

$$a_i = \frac{16\pi}{3^{3/2}} Z^4, \qquad c_i = b_i + 3, \qquad \frac{b_i}{\ln b_i} \approx \frac{4}{3^{1/2}\pi} \frac{Z^4}{Z-i} \left(\frac{2I_\mathrm{H}}{I_i}\right)^2. \tag{31}$$

Substituting (30) into (1) and ignoring the contribution of $k_{fe}{}^*(\nu) + k_s$, we obtain the following estimate for the Rosseland mean free path in a dense plasma:

$$l_{R,dp}[\mathrm{cm}] = 0{,}4 \frac{AT^3[\mathrm{keV}]}{\rho[\mathrm{g \cdot cm^{-3}}] a_i} \left[210 + 5b_i \left(\frac{I_i}{T}\right)^2 + \frac{c_i}{4} \left(\frac{I_i}{T}\right)^4\right]. \tag{32}$$

The error in (32) when (29) is satisfied should evidently be less than a factor $\sim$2–5. On the one hand, this is corroborated by direct comparison of Eq. (30) with quantum mechanical calculations of the photoionization cross section of various elements.[14] On the other, although it is in fact not necessary that the actual maximum cross section $\sigma_1^i(\nu)$, taking into account broadened and overlapping lines in the discrete spectrum (which comprise about half of the terms in the sum of oscillator strengths), be attained precisely at $h\nu = I_i$, it is clear that the difference between the frequency at the maximum and I_i/h cannot change the value of l_R significantly (by more than severalfold) when I_i/h lies in the vicinity of the maximum of the Rosseland function.

From the standpoint of photon absorption by bound

TABLE I. Comparison of Rosseland mean free paths calculated with different formulas for lead plasma at $T = 300$ eV.

$\rho\,\mathrm{g \cdot cm^{-3}}$	10^{-5}	10^{-2}	10^{-1}	1	10	10^2	10^3
$\bar{i}$	55.3	49.4	43.6	37.0	30.2	20.0	21.9
I_i/T	17.0	10.1	7.9	5.8	3.7	1.8	2.1
$l_{R,\,min}$, cm	38	$3.2 \cdot 10^{-2}$	$2.7 \cdot 10^{-3}$	$2.3 \cdot 10^{-4}$	$2.0 \cdot 10^{-5}$	$1.7 \cdot 10^{-6}$	$1.7 \cdot 10^{-7}$
$l_{R,\,dp}$, cm	$5.6 \cdot 10^2$	0.22	$1.4 \cdot 10^{-2}$	$8.3 \cdot 10^{-4}$	$5.2 \cdot 10^{-5}$	$3.6 \cdot 10^{-6}$	$3.8 \cdot 10^{-7}$
$l_{R,\,rp}$, cm	$2.8 \cdot 10^7$	36	0.51	$8.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-4}$	$5.0 \cdot 10^{-6}$	$5.6 \cdot 10^{-7}$

electrons, a dense plasma differs from a rarefied one in two important aspects: a) ionization equilibrium in a dense plasma is characterized by a lower value of I_i/T, the main contribution to the Rosseland mean coming from transitions out of the ground state; b) absorption lines are broader in a dense plasma, and give a larger contribution to the Rosseland mean free path (recall that infinitely narrow lines do not generally contribute to l_R). If by a dense plasma we mean one which satisfies (29), then by virtue these properties, it is precisely in a dense plasma that the fraction of the overall sum of oscillator strengths which gives the major contribution to l_R should be a maximum, and the estimate (21) of the minimum [see also (27)] is the closest to the actual value.

To demonstrate this result via a concrete example, we present in Table I the values of the Rosseland mean free path in lead, computed via Eqs. (21), (28), and (32) for $T = 300$ eV over a wide range of density. The mean ionization level $\bar{i} = \bar{i}(\rho, T)$ was computed with the aid of the generalized Raizer approximation, as in Ref. 7. Bearing in mind that "good agreement" of the computed values of the Rosseland mean free path means that they differ by only a small factor, we see from the table that in a dense plasma, with $1 \lesssim I_i/T \lesssim 5$, all these estimates are consistent with each other; in the low-density regime, with $I_i/T > 5$, the lower bound on l_R obtained in the present work is much smaller (by several orders of magnitude) than the actual values. Recall that the estimate (32) is not applicable in a low-density plasma, since (29) does not hold. The estimate (28) must be approached with a certain amount of caution, even in a very low-density plasma, since the contribution of discrete transitions was neglected in deriving it. Under these conditions, it would be preferable to use a much more complicated computational model, the modified Hartree-Fock-Slater model,[15] which takes into account both the actual structure of the excited states of multiply-charged ions and the actual line-broadening mechanisms.

We note in conclusion that Eq. (28), which was derived in Ref. 12 for a low-density plasma, also provides a fairly good description of the high-density case as well, when the mean ionization level $\bar{i}$ is determined from a more general ionization equation than the one in Ref. 16, which is applicable to a dense plasma, and the condition $I_i/T \gtrsim 1$ holds. In the limit $I_i/T \ll 1$, the error in (28) grows without bound, and only (32) should be used to give a realistic estimate of l_R.

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