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The Calculation of the Opacity of Hot Dense Plasmas

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Abstract

A review of the calculation of the radiative opacity of hot dense material is presented. An attempt is made to describe some of the approximations and assumptions implicit in current calculations and to indicate areas in which improvements may be made.

(Invited paper at the Second International Conference on the Radiative Properties of Hot Dense Matter)

1. Introduction

The calculation of photoabsorption by hot dense material was first of interest in astrophysical studies, particularly in the calculation of stellar structure. More recently a knowledge of the opacity of high-temperature air has been required (used for example in the calculation of atmospheric re-entry heat transfer) and in the last few years the opacity of laboratory (particularly laser-produced) plasmas has been of interest. Although these plasmas cannot always be considered to be in Local Thermodynamic Equilibrium (L.T.E.), the complex subject of the departure from L.T.E. is not considered here. However, much of the paper is relevant to both L.T.E. and non-L.T.E. plasmas.

Calculations of laboratory plasma opacities have presented different problems to those of astrophysical plasmas principally because of the much wider range of material involved. In particular whereas medium and high-Z elements occur as low concentration impurities in astrophysical situations, they are increasingly being considered as major constituents of laser- and ion-beam targets.

Because of the lack of experimental opacity data (except for cold material) calculated values have to be relied upon. Several excellent papers have appeared in the literature which have reviewed the subject (Huebner (1964), Cox (1965), Carson, Mayers and Stibbs (1968), Rozsnyai (1982)) and it is not the purpose of the present paper to go over this ground, but rather to bring out the underlying assumptions of the various methods used in opacity calculations and to suggest areas in which further work is still needed. In this paper we shall only consider temperatures which are sufficiently high that molecular absorption is negligible (a few eV) and photon energies low enough (less than about 1 MeV) that high-energy absorption processes such

as pair-production and nuclear photoabsorption can also be ignored. Only electronic transitions in the field of the ions are considered (bound-bound,bound-free and free-free) and these constitute the major absorption processes for most conditions of interest in both stellar and laboratory plasmas.

2. The one-electron average-atom model

Because the calculation of photoabsorption requires a knowledge of both the absorption strength of each species in the plasma as well as the concentration of that species, both a quantum-mechanical and statistical-mechanical description of the plasma is required. Instead of constructing a full quantum-statistical model, the usual approach has been to consider an 'average-atom' in the plasma. The calculation involves computing an average-atom potential from which a set of orbitals is obtained by solution of the one-electron wave equation. Non-integer populations are then assigned to each orbital and the 'one-electron' interaction with the radiation field is calculated. Finally account is taken of the departure from the average values occurring in a real plasma and in this way it is hoped that an approximation to a full quantum-statistical treatment is recovered. An opacity calculation therefore naturally divides into two parts; the first being the calculation of average one-electron quantities (orbital populations, orbital energies, oscillator strengths etc.) and the second ,which is less well understood, being the correction due to the distributions about the average values occurring in a real plasma.

Different workers have calculated the average-atom potential by a variety of methods. The screened-Coulomb potential is a popular choice because of its simplicity. Some of the quantum-mechanical properties of an electron in a Coulomb field can be expressed in a simple form (for example eigenvalues and orbital radii). Other properties have been calculated exactly, for example bound-bound electric-dipole oscillator strengths have been computed by Menzel and Pekeris (1935) and by Green, Rush and Chandler (1957),the bound-free and free-free Gaunt factors were given by Karzas and Latter (1961) while Naqvi (1964) gives expressions for Slater integrals of Coulomb

field orbitals. The use of a non-Coulomb potential was first considered by Grant (1958) and Green (1958) who looked at the calculation of free-free Gaunt factors. Carson, Mayers and Stibbs (1968) presented calculations of stellar opacities using a Thomas-Fermi average-atom potential from which numerical wavefunctions were calculated. There are in certain cases large differences between their opacity values and those calculated using a screened-Coulomb model. The calculation of free-free and bound-free photoabsorption cross-sections in different statistical potentials has been considered recently by Shalitin et al. (1982) and by Feng and Pratt (1982) for bound-free and by Green (1981), Lamoureux et al. (1982) and Feng et al. (1983) for free-free transitions. Rozsnyai (1972) and Liberman (1979,1982) have developed models in which average-atom orbitals are obtained using self-consistent-field procedures and such orbitals were used by Rozsnyai (1973) in calculations of bound-free photoabsorption cross-sections.

The screened-Coulomb model is still used extensively where speed of calculation is essential, an example being the XSN package (Lokke and Grasberger (1977)), which is designed to provide values of opacity in-line with target simulations. It is found to work least well when the temperature is low enough that only a small fraction of the electrons are ionised and the potential in the outer part of the atom is far from Coulombic. For example, the bound-bound oscillator strengths for $\Delta n=+1$ transitions calculated for Gold in a Coulomb and a Thomas-Fermi potential (figure 1) show that although for a temperature of 1 keV (where $Z^*/Z \sim 0.7$) the Coulombic and non-Coulombic oscillator strengths are very similar, at 100eV (where $Z^*/Z \sim 0.2$), the oscillator strengths calculated in the Thomas-Fermi potential are considerably lower for transitions involving the f and g orbitals which because of their non-penetrating character are particularly sensitive to the potential in the outer part of the atom. Further comparison between the use of Coulombic and non-Coulombic

potentials in the calculation of opacity can be found in the work of Carson and Hollingsworth (1968).

For low-Z elements of astrophysical interest, relativistic corrections to electronic motion are not large. However for high-Z elements of interest in laboratory plasmas, the effect of relativity is known to be important (Grant (1970)) and the inclusion of relativistic corrections to the Shroedinger equation or the use of the Dirac equation is required. The effect of relativity is to make one-electron orbitals more tightly bound. The effect becomes smaller the larger the principal quantum number and the energy of $\Delta n=+1$ transitions increases with increasing Z. Figure 2 shows the change for the 1s→2p transitions for which this increase is greatest. In the non-relativistic approximation the electric-dipole hydrogen-like oscillator strength is independent of Z. Rose (1982) shows that for $\Delta n=+1$ transitions the effect of relativity is to decrease the oscillator strengths of hydrogen-like ions and the effect is shown in figure 2 for the 1s→2p transitions.

The average-atom model allows non-integer orbital occupancies. Mayer (1947) noted that the energy of interaction between electrons cannot be taken as negligible and the usual statistics of independent fermions cannot be applied. Mayer (1947) (see also Green (1964), appendix 1) proved a high-temperature expansion for the probability of occupancy of orbital i, p_i, to be

$$p_i = \frac{1}{e^{\epsilon_i/kT - \eta} + 1} + 0\left[\left(\frac{H}{kT}\right)^2\right] .$$

The first term is just the independent electron expression with the eigenvalue ϵ_i appearing in place of the independent electron energy. The correction term involves some measure of the inter-electron interaction, denoted H. Green (1964), in a model problem and more recently More (1981),

in a set of more realistic calculations showed that the first term was a reasonable approximation to p_i over a range of H/kT.

In calculating the absorption strength resulting from a transition i→f, in addition to requiring knowledge of the orbital occupancy which for level i is simply $\omega_i p_i$, (where ω_i is the degeneracy of level i) it is also necessary to know the probability that there will be a hole in the final orbital f, q_f where

$$q_f = 1 - p_f \ .$$

The possibility $q_f \neq 1$ is always considered for bound-bound transitions. However it is not necessary for it to be considered for bound-free and free-free absorption unless the free electrons are degenerate. For photoabsorption involving a discrete edge, the multiplicative correction factor to the non-degenerate photoabsorption cross-section is just

$$q = \frac{1}{1 + e^{-(h\upsilon/kT - I) + \eta}} \ ,$$

where $h\upsilon$ is the photon energy and I is the ionisation potential of the level in question (figure 3). Free-free Coulombic Gaunt factors including the effects of degeneracy have been calculated by Green (1960).

3. Beyond the one-electron average atom model

The one-electron average-atom model is a very useful approximation because it allows opacity calculations to be performed in an acceptable length of time. However, because each one-electron orbital is associated with a single energy, the model predicts only one energy for each one-electron transition. In reality transitions occur between different energy levels of the ions in the plasma and in general many transitions, each occurring at a different energy, involve the same one-electron transition. It is possible to consider the transitions occurring between configurations or at a more detailed level, between terms resulting from the configurations. As first pointed out by Mayer (1947) this splitting of the one-electron transition energy is particularly important for the calculation of the Rosseland mean opacity which is very sensitve to 'windows' in the absorption spectrum. The contribution to the Rosseland opacity from a single line below an absorption edge can be considerably different from that of a number of different lines, slightly different from one another in energy, absorbing in roughly the same part of the spectrum. The same effect occurs for absorption edges; instead of one edge for each one-electron energy level, a number of edges slightly different in energy are found. With the exception of a few cases (for example the calculation of the opacity of air performed by Armstrong, Holland and Meyerott (1958) and calculations of the opacity of highly ionised iron where only H- and He-like ions have a significant abundance (Rozsnyai (1982)), 'term-splitting' has not been included and the usual method (Cox (1965), Carson, Mayers and Stibbs (1968), Argo and Huebner (1976)) is to consider transitions between different configurations. In order to calculate the contribution to the opacity of the transition between configuration α and β for which the orbital occupation numbers are

$$n_k^\alpha = n_k^\beta \qquad k \neq i \text{ or } f$$

$$n_i^\alpha = n_i^\beta + 1$$

$$n_f^\alpha = n_f^\beta - 1$$

it is necessary to know both the transition energy $\Delta E_{\alpha\to\beta}$ and also the probability of configuration α occurring in the plasma. The transition involves the one-electron jump i→f and has energy

$$\Delta E_{\alpha\to\beta} = I(f) - I(i) + \sum_k (n_k^\alpha - \delta_{ki})\left[H(f,k) - H(i,k)\right] \quad .$$

I(a) is the expectation value of the one-electron operator and for the non-relativistic case is given (in a.u.) by

$$I(a) = \langle a| -\tfrac{1}{2}\nabla^2 - \tfrac{Z}{r} |a\rangle \quad .$$

H(a,b) is the average-of-configuration interaction energy between an electron in shell a and one in b and is given for non-relativistic orbitals by

$$H(a,b) = F^0(a,b) - \tfrac{1}{2}\sum_{k\geq 0}^{\delta_{a,b}} \left(\frac{\omega_a}{\omega_a - \delta_{a,b}}\right) \begin{pmatrix} l_a & k & l_b \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(a,b) \quad ,$$

where $F^k(a,b)$ and $G^k(a,b)$ are the usual Slater integrals. Some workers do not include the terms for which k>0, approximating the interaction by the direct spherically symmetric term. For screened-Coulombic calculations the interaction energy is approximated by the use of screening constants. The probability of an ion being found in configuration α can be evaluated from the statistical-mechanical expression (Cox (1965), More (1983))

$$P(\alpha) = \frac{D_\alpha \exp\left[-\dfrac{E(\alpha) + F}{kT}\right]}{\sum_\alpha D_\alpha \exp\left[-\dfrac{E(\alpha) + F}{kT}\right]} \quad .$$

The degeneracy factor D_α is simply

$$D_\alpha = \prod_i \frac{\omega_i!}{n_i^\alpha!\,(\omega_i - n_i^\alpha)!} \quad .$$

$E(\alpha)$ is the energy of an ion in configuration and F is the free energy of the n^{α}_{free} free electrons in the average atomic volume where

$$n^{\alpha}_{free} = Z - \sum_{k} n^{\alpha}_{k} .$$

A simpler expression has been used, for example, by Carson, Mayers and Stibbs (1968)

$$P(\alpha) = \prod_{i} \frac{\omega_i !}{n_i^{\alpha} ! \, (\omega_i - n_i^{\alpha}) !} \, p_i^{n_i^{\alpha}} q_i^{\omega_i - n_i^{\alpha}}$$

which assumes that the electrons are not statistically correlated. The subject of statistical correlation between electrons in a partially ionised plasma has been investigated by Green (1964) and Grimaldi (1983).

There are plainly several areas in which further work needs to be performed. The most obvious is that of the inclusion of term-splitting. In this context it is worthwhile to note that Moszkowski (1962) has given a general expression for the distribution of lines resulting from term-splitting. Secondly configuration-interaction has not yet been included in any opacity calculation. It is expected that this will predict the appearance of one-photon two-electron absorption processes and detailed calculations are needed to assess their effect. Finally the error incurred because the average-atom orbital set is not optimal for any of the levels in the plasma has not been investigated. The effect of this is expected to become more important as the number of bound electrons increases and could be assessed by comparison between average-atom and Hartree-Fock calculations. With the inclusion of all of these effects, the simplicity gained by starting with a one-electron average-atom model may be lost and it may prove easier to begin the opacity calculation with individual ionic structure calculations.

4. Spherical symmetry

In average-atom opacity calculations the appoximation is made that the effects of plasma neighbours can be represented as a spherically symmetric alteration to the central potential. One possible improvement is to solve the wave equation in the field of more than one fixed nucleus and then average over the possible nuclear positions. The electrons are then shared between more than one ion. This approach has been investigated by Rose (1983) who shows that consideration of transitions of an electron in the field of more than one nucleus predicts contributions to the opacity not arising in the usual single-centre treatment which couple radiation to ionic kinetic energy. The multi-centre analysis also leads to the prediction of photoabsorption occurring by an electron making a transition from an orbital centred mainly on one nucleus to one centred principally on a neighbouring one. Such 'charge-transfer' transitions are also not predicted by the usual single-centre analysis. Detailed calculations of these effects have still to be performed.

5. Conclusions

In this paper it has not been possible to cover every aspect of the calculation of opacities and many important topics, such as the subject of line-shapes, have not been mentioned. It has been shown however that although much progress has been made there are still areas of uncertainty particularly regarding how to include accurately the variety of ions existing in the plasma and also how to treat neighbouring plasma particles. Although accurate values of opacity are needed for many applications there still remain many uncertainties in the modelling and without experimental information it is very difficult to assess their importance.

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Figure captions

Figure 1. One-electron relativistic electric-dipole oscillator strengths for Gold calculated using Coulombic and non-Coulombic potentials.

Figure 2. The dependence of the fractional increase in transition energy $(\Delta E_R - \Delta E_{NR})/\Delta E_{NR}$ and of the electric-dipole oscillator strength f on the nuclear charge Z for the $1s_{1/2} \rightarrow 2p_{1/2}$ and $1s_{1/2} \rightarrow 2p_{3/2}$ hydrogen-like transitions.

Figure 3. The dependence of q (the correction factor to the non-degenerate photoelectric cross-section) on degeneracy parameter η and on ionised electron energy $h\nu$-I.

FIGURE 1.

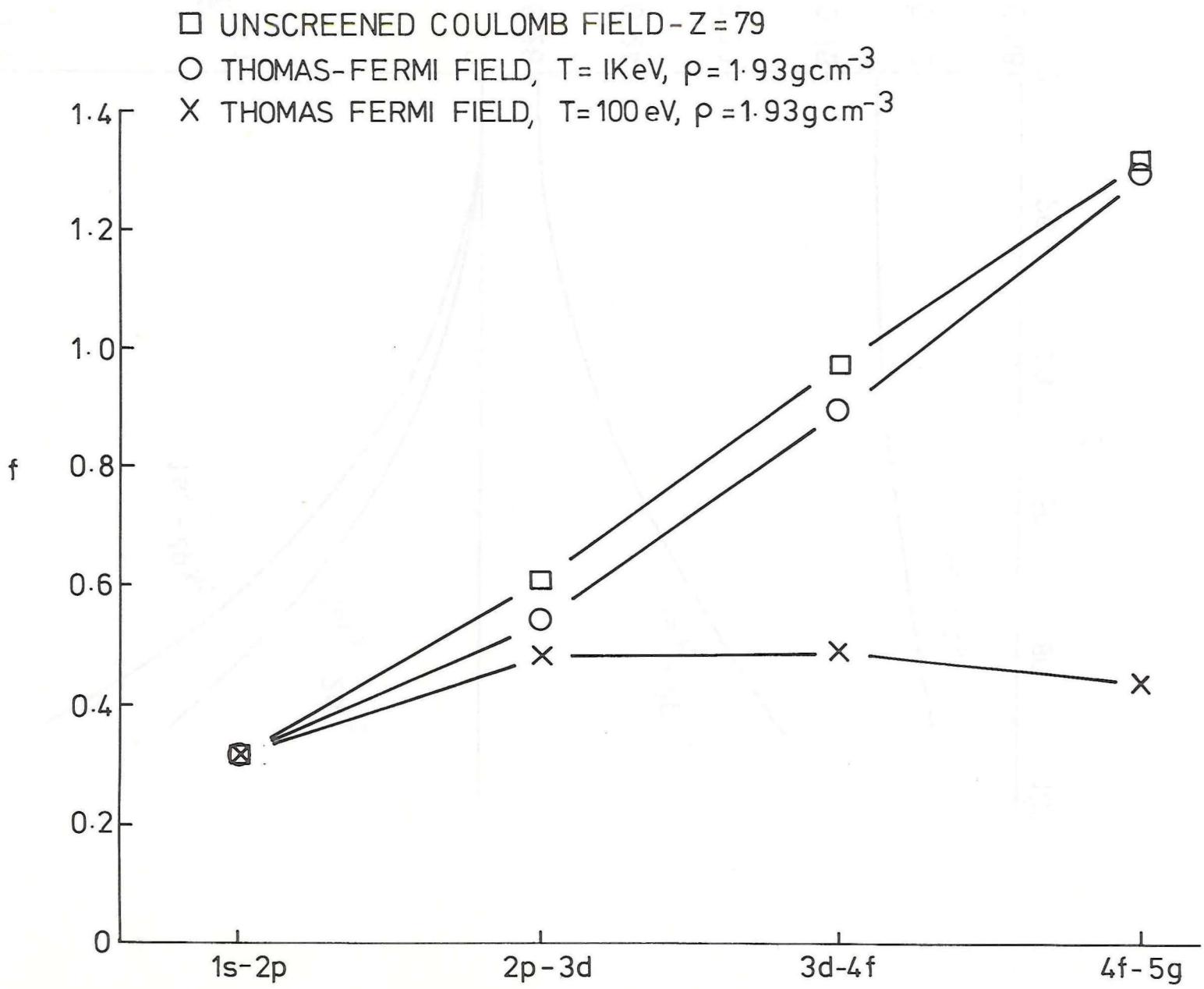
□ UNSCREENED COULOMB FIELD - Z = 79
○ THOMAS-FERMI FIELD, T = 1KeV, ρ = 1·93gcm⁻³
X THOMAS FERMI FIELD, T = 100 eV, ρ = 1·93gcm⁻³
f
1·4
1·2
1·0
0·8
0·6
0·4
0·2
0
1s-2p
2p-3d
3d-4f
4f-5g

FIGURE 2.

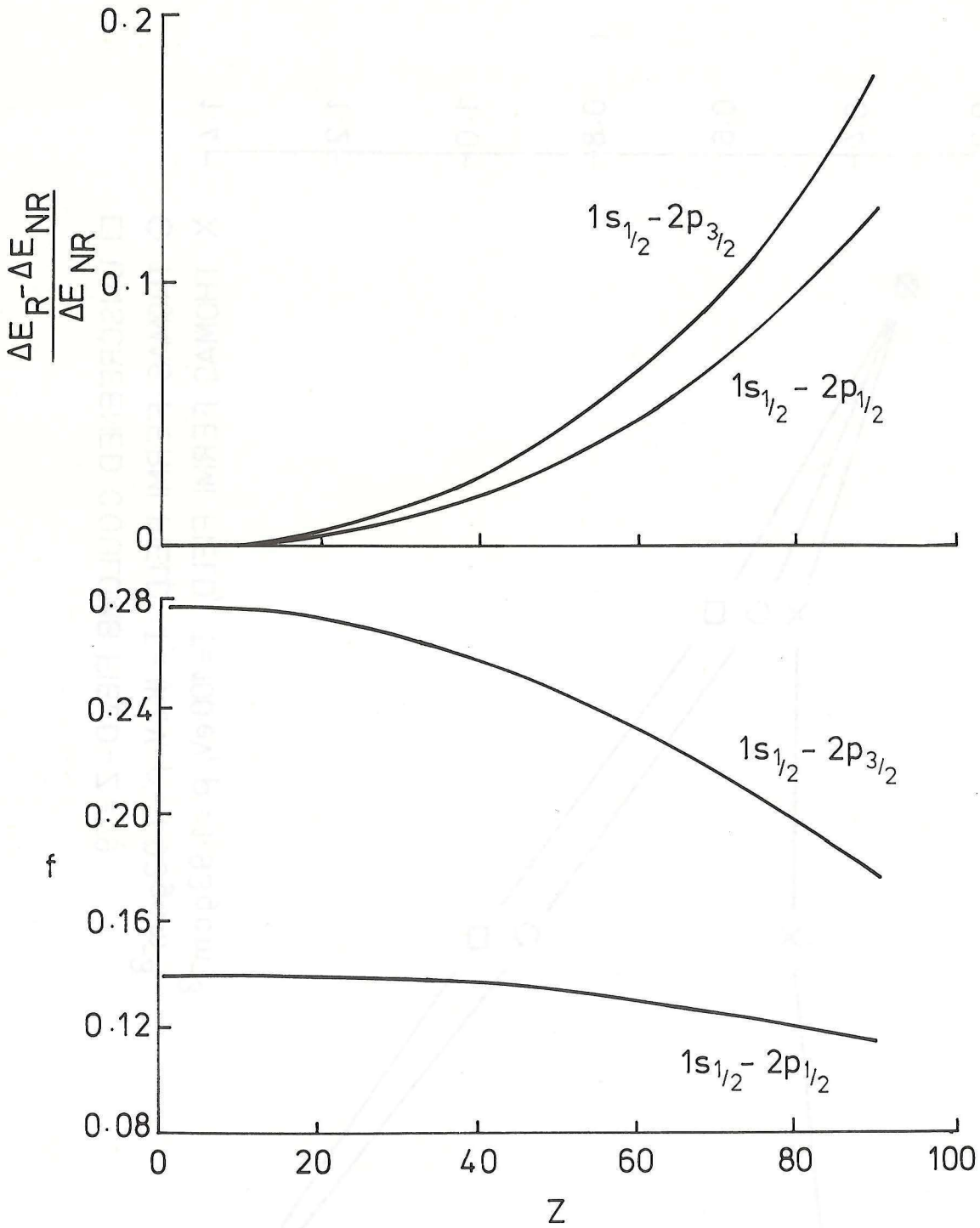
0·2
0·1
0
$\frac{\Delta E_R - \Delta E_{NR}}{\Delta E_{NR}}$
$1s_{1/2} - 2p_{3/2}$
$1s_{1/2} - 2p_{1/2}$
0·28
0·24
0·20
0·16
0·12
0·08
f
$1s_{1/2} - 2p_{3/2}$
$1s_{1/2} - 2p_{1/2}$
0
20
40
60
80
100
Z

FIGURE 3