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Radiation pressure and the Thomas–Fermi equation of state

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Abstract. This paper studies the interaction of radiation with matter in a high-temperature environment. The radiation pressure is calculated carefully, including the coupling to the high-density electron plasma. The calculation yields a correction to the expression for radiation pressure given by Inman. The results are applied to investigate whether radiation pressure can produce significant alterations of the electron density in atoms.

1. Introduction

This paper studies the interaction of radiation with matter in a high-temperature environment such as a stellar interior or the core of a highly compressed laser-fusion pellet target. According to a well known rule for the equation of state of hot dense matter (Zel'dovich and Raizer 1966, Cox and Giuli 1968, Bond *et al* 1965), the total pressure is computed as the sum of independent contributions corresponding to radiation, electrons and ions ($p = p_r + p_e + p_i$). Obviously, this rule is only an approximate treatment of a complicated situation, and it is desirable to determine the limits of the additive rule or corrections to it. The result obtained below is a correction to the additive rule which occurs because of the interaction of radiation with the electron gas.

The radiation pressure is not simply the black-body pressure ($4\sigma/3cT^4$), because at high densities the electron plasma modifies the photon group velocity and density of states. The radiation pressure is carefully calculated in § 2 (including the plasma effect); because of a subtle point, our result for the radiation pressure differs from that given by Inman (1965).

At high temperatures the radiation pressure may be larger than the electron or ion pressures and some fraction of this radiation pressure will act upon the electron distribution. The radiation pressure will tend to collapse or compress the electron distribution, because part of the radiation spectrum is excluded from the dense electron gas in the atomic core. This effect is studied in § 3 and shown to be very small at temperatures below 10^9 K.

The electron pressure is conveniently calculated by Thomas–Fermi theory for atoms that are not totally ionized (Latter 1955, Feynman *et al* 1949). The ion pressure may be approximately determined from ideal-gas formulae or more accurately from numerical calculations for the one-component plasma (Brush *et al* 1966, Hansen 1973). An approximate treatment of the coupling of electron and ion contributions was recently given by More and Skupsky (1976).

This paper concentrates on the interaction of radiation with electrons in thermal equilibrium. One effect of radiation is to promote electrons to excited states but this is already included in the finite-temperature Thomas–Fermi theory. The mechanism considered in § 3 is an additional effect in which radiation alters the wavefunctions of electron states and thereby alters the electron charge density. Alternately phrased, some fraction of the radiation pressure is transmitted to the electron distribution and tends to compress the atom.

The calculation given below is an approximate treatment which extends the development of Thomas–Fermi theory from the viewpoint of the inhomogeneous electron gas (Kohn and Hohenberg 1965). A free-energy function is constructed for radiation in the presence of a uniform electron gas and this is adapted to the atomic structure problem via the local density approximation. The approximation is probably not highly accurate (no more so than the usual Thomas–Fermi approximation), but it is sufficient to demonstrate the (small) magnitude of the effects.

2. Radiation pressure (uniform gas)

This section calculates the pressure of black-body radiation in the presence of an electron plasma having constant (uniform) number density n_e. The radiation free energy $\mathscr{F}_r$ of equation (1) agrees with an expression given by Inman (1965), but the formula for the radiation pressure p_r does not agree.

For transverse plasma waves with frequency $\omega = \omega(\boldsymbol{k})$ and zero chemical potential, the density of Helmholtz free energy is (Landau and Lifshitz 1966):

$$\mathscr{F}_r = -2k_BT\int \ln(1-e^{-\hbar\omega(\boldsymbol{k})/k_BT})\frac{d^3k}{(2\pi)^3} \tag{1}$$

where $\boldsymbol{k}$ is the wavevector and k_B is the Boltzmann constant. The factor 2 prefixing the integral corresponds to the sum over photon polarizations transverse to the wavevector.

The dispersion relation for transverse plasma waves is:

$$\omega(\boldsymbol{k}) = (\omega_p^2 + c^2k^2)^{1/2} \tag{2}$$

where the plasma frequency ω_p is determined by the electron number density n_e according to:

$$\omega_p = (4\pi n_e e^2/m_e)^{1/2}.$$

The free-energy density is evaluated by inserting (2) into (1) and integrating by parts. The result is then:

$$\mathscr{F}_r = -\frac{(k_BT)^4}{3\pi^2\hbar^3c^3}B_{3/2}(x_0) \tag{3}$$

where $x_0 = \hbar\omega_p/k_BT$ and the function $B_{3/2}(x_0)$ is defined by

$$B_{3/2}(x_0) \equiv \int_{x_0}^{\infty} \frac{(x^2-x_0^2)^{3/2}}{e^x-1}\,dx. \tag{4}$$

For the limiting case of low electron density, $x_0 \to 0$ and $B_{3/2}(0) = \pi^4/15$. In this case, equation (3) is a standard result for black-body radiation (Landau and Lifshitz

1966). As x_0 rises, $B_{3/2}(x_0)$ decreases from the initial value $\pi^4/15$; series expansions for the free energy are given by Inman (1965). Table 1 gives numerical values for the functions $B_{3/2}$ and $B_{1/2}$ (defined below).

Table 1.

x_0	$B_{3/2}(x_0)$	$B_{1/2}(x_0)$	$\frac{3}{2}x_0^2B_{1/2}/B_{3/2}$
0	6·4939	1·6447	0
0·5	6·0336	1·0563	0·0657
1·0	5·0894	0·6895	0·2032
1·5	4·0514	0·4503	0·3751
2·0	3·0997	0·2932	0·5675
2·5	2·3029	0·1900	0·7735
3·0	1·6724	0·1225	0·9892
3·5	1·1924	0·0786	1·2119
4·0	0·8375	0·0502	1·4400
4·5	0·5808	0·0320	1·6720
5·0	0·3986	0·0203	1·9072
5·5	0·2710	0·0128	2·1447
6·0	0·1828	0·0081	2·3842

Inman computes the total free energy of radiation F_r as the volume integral of the density $\mathcal{F}_r$, so that for the uniform system one has $F_r = V\mathcal{F}_r$. He then evidently computes the pressure by differentiation with respect to V, finding the result $p_r = -\mathcal{F}_r$ for the radiation pressure.

The work of the next section leads to a *different* final expression for the radiation pressure which is already suggested at this stage by the observation that Inman has performed the differentiation with respect to volume at constant electron density $n_e = N_e/V$. However the radiation cannot be compressed independently of matter. If instead the electron density is allowed to change with volume V (keeping N_e constant), the pressure becomes:

$$p_r = -\mathcal{F}_r + \frac{2}{\pi}\frac{e^2}{\hbar c}\frac{(k_B T)^2}{mc^2} n_e B_{1/2}(x_0) \tag{5}$$

or

$$p_r = -\mathcal{F}_r\left(1 + \frac{3}{2}x_0^2\frac{B_{1/2}(x_0)}{B_{3/2}(x_0)}\right)$$

where

$$B_{1/2}(x_0) \equiv \int_{x_0}^{\infty} \frac{(x^2 - x_0^2)^{1/2}}{e^x - 1}\,dx \tag{6}$$

is also given in table 1.

For large values of x_0, the radiation pressure of equation (5) differs significantly from the formula given by Inman and so it appears worthwhile to be certain that (5) is correct. A very clear justification for equation (5) is provided by the calculations of the next section.

3. Modified Thomas–Fermi theory

The radiation free energy of equation (3) is now combined with the electronic free energy to generate a modified version of the Thomas–Fermi theory. The calculation supplies an additional justification for the radiation pressure formula of equation (5) and also indicates the extent to which radiation pressure is able to alter the charge distribution within an atom.

The Helmholtz free energy per electron of a uniform non-interacting electron gas at density n will be denoted $f(n, T)$. The explicit form of $f(n, T)$ is a well known expression involving Fermi–Dirac integrals and is quoted below.

As is conventional in Thomas–Fermi theories, space is divided into spherical cells surrounding the nuclei (Latter 1955, Feynman *et al* 1949, Brush *et al* 1966). The total free energy of one ion sphere containing a positive nuclear charge $+Ze$ and an electron density $n(r)$ is approximately given by:

$$F[n(r)] = \int n(r) f(n(r), T)\, \mathrm{d}^3r + \frac{e^2}{2} \int \frac{n(r)n(r')}{|\boldsymbol{r}-\boldsymbol{r}'|}\, \mathrm{d}^3r\, \mathrm{d}^3r' - \int \frac{Ze^2 n(r)}{|\boldsymbol{r}|}\, \mathrm{d}^3r + \int \mathscr{F}_{\mathrm{r}}(n(r))\, \mathrm{d}^3r. \tag{7}$$

The first three terms occur in the standard finite-temperature Thomas–Fermi theory and the last term represents the analogous treatment of radiation. The first term is the free energy associated with free-electron kinetic energy (explicit form given below). The second and third terms are the electron–electron interaction, neglecting exchange and correlation, and the electron–nucleus interaction. The local density approximation is used in the first and fourth terms; the non-uniform gas is treated by adding contributions for the uniform gas evaluated at the local density $n(r)$.

The local density approximation would be accurate if the density gradients were small, and the approximation is being applied outside its formal domain of validity in any application to atomic structure. Nevertheless the Thomas–Fermi theory gives a useful account of the general properties of high-density matter and it appears reasonable to use this approximation to estimate the radiation effects. If the results corresponded to a larger effect, it would be interesting to attempt a more accurate calculation.

The free energy $F[n(r)]$ is defined for an arbitrary electron density but should take on a minimum value for the correct density. Variations of $n(r)$ are subject to the constraint

$$\int n(r)\, \mathrm{d}^3r = Z$$

where this integral also runs over the ion sphere. The constraint is enforced by introducing a Lagrange multipler μ which is the electron chemical potential. The condition that $F[n]$ be a minimum yields the equation:

$$\mu = \frac{\delta F}{\delta n(r)} = f + n\frac{\partial f}{\partial n} - eV(r) + \mu_{\mathrm{er}}(r) \tag{8}$$

where $V(r)$ is the total electrostatic potential determined by

$$V(\boldsymbol{r}) = \frac{Ze}{|\boldsymbol{r}|} - e\int \frac{n(r')\, \mathrm{d}^3r'}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

and $\mu_{er}(r)$ is the contribution of radiation to the electron chemical potential, determined by:

$$\mu_{er}(r)=\frac{\partial \mathscr{F}_r}{\partial n}=\frac{2}{\pi}\frac{e^2}{\hbar c}\frac{(k_B T)^2}{mc^2}B_{1/2}(x_0(r)) \tag{9}$$

with $x_0(r)=\hbar\omega_p(r)/k_B T$ and $\omega_p(r)=(4\pi n(r)e^2/m_e)^{1/2}$.

The electron density is determined by the requirement that the left-hand side of equation (8) be independent of position although the individual terms on the right are not. If the radiation contribution $\mu_{er}(r)$ is omitted, then equation (6) is equivalent to the usual Thomas–Fermi theory. The term μ_{er} therefore governs the alteration of the electron distribution by radiation.

This effect may be interpreted as follows: radiation energy of any specified frequency ω is excluded from the central parts of the atom where the electron density is so high that the local plasma frequency $\omega_p(r)$ exceeds ω. In this way, a fraction of the radiation pressure is transmitted to the electron distribution.

The electron chemical potential μ is spatially constant across the atomic volume as a condition of equilibrium and therefore $\nabla\mu=0$ or

$$0=\left(2\frac{\partial f}{\partial n}+n\frac{\partial^2 f}{\partial n^2}\right)\nabla n+\nabla\mu_{er}-e\nabla V.$$

We will multiply this equation by $n(r)$ and then use equation (9) to replace the term $n\nabla\mu_{er}$ by $-\nabla\mathscr{F}_r+\nabla(n\mu_{er})$. The result may then be rewritten in the form of a familiar condition for equilibrium:

$$\nabla p_{tot}=-en(r)E(r) \tag{10}$$

where the electric field is $\boldsymbol{E}(r)=-\nabla V(r)$ and the total pressure p_{tot} is

$$p_{tot}(r)=n^2\frac{\partial f}{\partial n}-\mathscr{F}_r+n(r)\mu_{er}(r). \tag{11}$$

Equation (11) is the only expression for the total pressure compatible with equation (10), up to an uninteresting constant. The first term in equation (11) is the usual expression for the electron pressure in the Thomas–Fermi theory, as shown below. The second term $-\mathscr{F}_r$ is the Inman expression for the radiation pressure, and the third term is precisely the correction found in equation (5). This last term is a modification to the total pressure associated with the interaction of radiation and electrons.

In order to verify that the first term of equation (11) is the usual electron pressure, it is useful to recall the well known form of $f(n, T)$, the free energy per electron of a uniform electron gas. The equation gives f in terms of an auxiliary quantity $\eta(r)$:

$$f=-k_B T\left(\eta+\frac{2}{3}\frac{F_{3/2}(\eta)}{F_{1/2}(\eta)}\right) \tag{12}$$

where η is determined from the local density n by:

$$n=\frac{4}{\sqrt{\pi}}\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}F_{1/2}(\eta) \tag{13}$$

and the Fermi–Dirac integrals $F_{1/2}$, $F_{3/2}$ are defined by

$$F_j(\eta)\equiv\int_0^\infty \frac{x^j\,dx}{1+\exp(x+\eta)}. \tag{14}$$

Using $dF_{3/2}/d\eta = -\frac{3}{2}F_{1/2}$, one can readily show that

$$n^2\frac{\partial f}{\partial n} = \frac{8}{3\sqrt{\pi}}k_BT\left(\frac{2\pi mk_BT}{h^2}\right)^{3/2}F_{3/2}(\eta)$$

and this is the usual Thomas–Fermi formula for the electron pressure.

There is still another derivation of the total pressure formula of equation (11), again differentiating the free energy with respect to volume but now performing the calculation within the ion-sphere picture. When a substance changes volume, each ion sphere changes volume by $d\Omega$. The neutrality condition is true at both volumes Ω_0 and $\Omega_0 + d\Omega$, which yields:

$$\int_{\Omega_0} \delta n(r)\, d^3r = -n(R_0)\, d\Omega = -n(R_0)4\pi R_0^2\, dR_0$$

where $\delta n(r)$ is the change in $n(r)$ produced by the small volume change and $n(R_0)$ is the number density at the ion-sphere boundary. Using equations (6) and (7), one can easily establish

$$\delta F = -p_{\text{tot}}\, d\Omega$$

where again p_{tot} is determined by equation (11), evaluated at $r = R_0$. Thus $p_{\text{tot}}(R_0)$ determines the bulk pressure of the substance.

The changes in electron density induced by the interaction with radiation are obviously very small. The correction to the pressure may be written

$$\delta p = n\mu_{\text{er}} = nk_BT\frac{2}{\pi}\frac{e^2}{\hbar c}\frac{k_BT}{mc^2}B_{1/2}(x_0)$$

where $e^2/\hbar c$ is 1/137·037, $B_{1/2}$ is of order unity (see table 1) and since normally $k_BT \ll mc^2$, this term is a very small correction to the electron gas pressure which is greater than or equal to nk_BT. (The term δp is not necessarily small with respect to the radiation pressure $-\mathcal{F}_r$ obtained by Inman.) At higher temperatures, where the effect would be more appreciable, a relativistic treatment would be required.

The smallness of this alteration of the electron density distribution therefore provides a verification of the additive pressure rule.

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