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1. DENSE ATOMIC PLASMAS (INTRODUCTION)

When a solid target is irradiated by an intense pulse of laser light, an inhomogeneous plasma is created (Fig. 1). A low-density ideal plasma ($n_e < 10^{21} \text{ cm}^{-3}$) expands toward the laser; this hot blowoff region refracts and absorbs the laser beam. The absorbed energy is conducted into a dense plasma region ($n_e = 10^{21}$ to 10^{23} cm^{-3}) where the heat flow is converted into hydrodynamic motion of the exploding plasma. The large reaction pressure shocks the target surface, compressing it above the initial solid density into a state which may be called high-density matter ($n_e > 10^{23} \text{ cm}^{-3}$).

The objective of inertial-confinement fusion research is to achieve energy production in deuterium-tritium fuel compressed by implosion to extreme densities up to 10^2 - 10^3 times the normal (cryogenic) liquid.¹ These densities are so much greater than those encountered in previous fusion plasmas that they raise many unique questions of atomic physics.²

High-density conditions cause dramatic changes in the physical mechanisms which govern most plasma energy-transport and coupling coefficients. It emerges that these coefficients are more sensitive to atomic properties in the dense plasmas.

Conversely, random electric fields in the dense plasma environment significantly perturb atomic bound electrons. When the plasma field exceeds the nuclear field, electrons are liberated from occupied ion-core states by an important process called pressure ionization.²⁻⁵

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Implosion experiments diagnosed by broadening of neon or argon emission lines show plasma electron densities in the range 10^{23} to 10^{24} cm^{-3} (Yaakobi et al.⁶; Hauer, Mitchell et al.⁷; Kilkenny, Lee et al.⁸). The analysis of line widths and intensity ratios is an important specialized branch of the atomic physics of dense plasmas (Griem,⁹ Hooper et al.,¹⁰ Hauer,¹¹ and Key¹²).

Fig. 1 Schematic representation of laser-irradiated flat target, showing a wide range of density-temperature conditions.

Typical inertial fusion targets are composed of a variety of materials (glass, neon, argon, nickel, plastic, gold) in addition to hydrogen isotopes; this means that we are interested in partially-ionized heavy atoms. For these materials, non-LTE effects are often very substantial. LASNEX simulations of recent gold-disk experiments show that the observed output of 2 keV x-rays is in agreement with non-LTE simulations but falls two orders of magnitude lower than an LTE calculation would predict.¹³ A special characteristic of non-LTE in laser-fusion plasmas is a finite or large optical depth.

The high density and significant optical depth of laser plasmas lead to a characteristic problem: it is difficult to make accurate or detailed observations of events occurring in the pellet implosion core. This circumstance compels us to rely heavily upon theory, which is tested primarily by its logical consistency and by overall agreement between experiment and a comprehensive target-implosion simulation.¹⁴

We can identify three levels of increasing sophistication in the theory of atomic processes in dense plasmas. In the most naive work, it is assumed that atomic rates are proportional to the densities of reacting particles; e.g., electron-impact ionization $\propto n_e$, three-body recombination $\propto n_e^2$, etc. For low-density plasmas, this approach gives well-known and widely-accepted results. At high density, it predicts qualitatively incorrect results, such as complete recombination.

A better strategy is to recompute both eigenstates and cross-sections in a density-dependent model potential, such as the Debye-Hückel or ion-sphere potentials. Calculations at this level include the most important high-density effects: pressure ionization, continuum lowering and free-electron degeneracy. Although the results are more reasonable, this approach leaves many unanswered questions about the fundamental physics.

At the third level of sophistication, attention is directed toward the discrete atomic character of the plasma environment. For each process, a rate is calculated and then averaged over the probable positions of neighboring ions. For example, the rate of electron-ion elastic collisions is expressed as an integral over the ion pair-distribution function (see Eq. 3-2). For static ion Stark-broadening of emission lines, the line profile reduces to a transform of the plasma microfield distribution.¹⁰

The third approach can also encompass non-static effects associated with a time-varying atomic environment; such effects have proven important in line-broadening theory.^{9,10}

At present, not many plasma rate coefficients are calculated at the third level of sophistication, but that is our ultimate objective. In order to build toward this goal, we need information about the structure of partially-stripped ions, their pairwise interactions and the average ion-ion correlations which result from thermal motion of the ions.

2. ION CORES--STRUCTURE, INTERACTIONS, AND CORRELATIONS

The ion core is a nucleus of charge Z together with $Z-Q$ tightly bound electrons. It is surrounded by loosely bound electrons, free electrons and neighboring ions.

For isolated ions, electron eigenvalues and ionization potentials can be calculated by self-consistent field methods. Data is available for a large number of groundstate ions.¹⁵

For many practical applications, it is adequate to use results from the Thomas-Fermi theory.¹⁶ The TF model of the isolated groundstate ion is a nucleus surrounded by a semiclassical elec-

tron gas distributed in a self-consistent potential. The TF electron distribution gives the ion a finite radius $R(Z,Q)$.

One advantage of Thomas-Fermi theory is a scaling law which relates different atomic species so that ion core properties depend only on the fractional charge Q/Z . For example, the TF ion radius $R(Z,Q)$ is scaled by

$$R(Z,Q) = Z^{-1/3} R_0(Q/Z) \quad (2-1)$$

This gives the radius of any ion in terms of a universal scaling function $R_0(x)$. Other atomic properties also scale, for example:

$$\text{total ion binding energy } E_{TOT} = Z^{7/3} E_0(Q/Z)$$

$$\text{ionization potential } I = Z^{4/3} I_0(Q/Z)$$

$$\text{ion dipole polarizability } \alpha = 1/Z \alpha(Q/Z)$$

$$\text{average ionization-excitation energy } \bar{I} = Z I_0(Q/Z)$$

Appendix A gives more complete definitions and limiting analytic forms for highly stripped ions. Table 1 gives the TF scaling functions in numerical form; it is remarkable that one can summarize the main properties of the ~4000 ions of the periodic chart on a single page.

How accurate is this Thomas-Fermi data? It is good enough for qualitative estimates, and even some quantitative applications, but not accurate enough to satisfy most theorists. Thomas-Fermi calculations are especially questionable for highly ionized ($Q/Z \rightarrow 1$) and neutral ($Q/Z \rightarrow 0$) limits. We can compare ionization potentials computed with the Thomas-Fermi theory to those obtained from relativistic self-consistent field calculations¹⁵ (Fig. 2): for light atoms there are disagreements of 50 to 100% while for heavy atoms the TF numbers are reasonably accurate.

The average ionization-excitation energy $\bar{I}(Z,Q)$ is used in the Bethe theory of fast-ion stopping¹⁶ to calculate energy transfer to bound electrons; this theory is extended to ion energy-loss in hot plasmas by Nardi, Peleg and Zinnamon.¹⁷ For cold matter, the experimental values of $\bar{I}$ are ~50% larger than the Thomas-Fermi result $\bar{I}(Z,0) \sim (6.5 \text{ eV})Z$. The same correction factor (~1.5) brings the TF function $I(Z,Q)$ into approximate agreement with quantum calculations for aluminum ions ($Q = 1$ to 13) performed recently by E. McGuire.¹⁸ The Bethe theory is limited to high projectile ion velocities; the low-velocity range may be treated by extension of the Lindhard-Winther theory² using recent calcu-

Table 1. Properties of Thomas-Fermi groundstate ions.²⁰
The numbers are scaled to $Z = 1$.

Q/Z	$\bar{I}_0$ (eV)	I_0 (eV)	E_0 (eV)	R_0 (Å)	α_0 (Å ³)
0.1	8.951	0.280	-20.908	5.141	36.006
0.2	11.526	0.882	-20.852	3.267	7.581
0.3	14.374	1.826	-20.720	2.365	2.390
0.4	17.694	3.210	-20.472	1.795	0.861
0.5	21.744	5.206	-20.058	1.383	0.318
0.6	26.953	8.147	-19.400	1.061	0.112
0.7	34.190	12.736	-18.374	0.791	0.0342
0.8	45.664	20.851	-16.739	0.552	7.608×10^{-3}
0.9	69.991	40.336	-13.859	0.321	7.362×10^{-4}

lations of electron-gas stopping due to Skupsky, Arista and Brandt, and Deutsch.¹⁹ Ion stopping is important both for calculations of heavy-ion fusion and for analysis of thermonuclear burn.²⁰

For non-degenerate plasmas, the equilibrium (LTE) ionization state $Q(\phi, T)$ can be estimated using an approximate version of the Saha equation:

$$-I(Z, Q) = \mu = kT \log \left(\frac{n_e \lambda_e^3}{2} \right) \quad (2-2)$$

$I(Z, Q)$ is obtained from Table 1, μ is the chemical potential for non-degenerate electrons, n_e is the free electron density, and

$$\lambda_e = \sqrt{\frac{h^2}{2\pi m k T}} = 6.92 \times 10^{-8} \text{ cm} \sqrt{\frac{1 \text{ eV}}{kT}} \quad (2-3)$$

is the electron thermal deBroglie wavelength. Equation (2-2) is only a rough approximation; a more accurate analytic formula for $Q(\phi, T)$ is given in Ref. 2 (Table III-1).

The ion radii in Table 1 can be used to estimate the plasma density at which ions touch their neighbors:

$$\rho = \frac{AM}{\frac{4\pi}{3} [R(Z, Q)]^3} \quad (2-4)$$

where A = atomic weight, M_p = atomic mass unit. This equation gives a reasonably accurate prediction of the charge state $Q(\rho)$ in the low-temperature degenerate range; i.e., it is a simple model for pressure-induced ionization.

At densities lower than that given by Eq. (2-4), ions come into close contact only during a collision. We are interested in the ion pair-potential $U(R)$ which governs ion-ion collisions.

Ion Interactions

The ion pair-potential can be written generally as

$$U(R) = \frac{Z_1 Z_2 e^2}{R} \phi(R) \quad (2-5)$$

where Z_1, Z_2 = nuclear charges and R = internuclear separation. The screening function $\phi(R)$ approaches unity when the ion separation R approaches zero. For large radii, ions interact through their effective charges and $\phi(R) \rightarrow Q_1 Q_2 / Z_1 Z_2$.

The pair-potential is defined as the groundstate energy of the electron-ion system at separation R minus the groundstate energy at infinite separation. In Thomas-Fermi theory, the screening function also has a scaling property; for similar ions ($Z_1 = Z_2$, $Q_1 = Q_2$) this reads $\phi = \phi(Q/Z, Z^{1/3}R)$.

Several authors have considered pair potentials for collisions of Thomas-Fermi atoms. Variational bounds for $U(R)$ are derived by Firsov (1957, 1958) and an approximate representation of the screening function $\phi(R)$ for collisions of neutrals is given by Lindhard, Nielsen, and Scharff (1963).²² Lee, Longmire and Rosenbluth²³ calculate $U(R)$ for identical neutral TF atoms at seven radial separations (see Table 2) from numerical solutions of the two-center Thomas-Fermi problem.

Fig. 2 Scaled ionization potentials for thirty elements fall into the shaded region.^{2,15} The solid line is the Thomas-Fermi ionization potential. Triangles, circles and squares respectively represent aluminum, iron and gold ionization potentials.

Table 2. Comparison of Screening Function $\phi(R)$ for Collisions of Neutral TF Atoms (Scaled to $Z_1 = Z_2 = 1$).

Radius R (Å)	$\phi(R)$ Lee, Longmire, Rosenbluth	$\phi(R)$ Superposition Approximation
0.029	0.900	0.892
0.059	0.818	0.812
0.117	0.693	0.690
0.234	0.520	0.521
0.468	0.318	0.327
0.927	0.178	0.154
1.874	0.041	0.051

In order to calculate the potential between ion cores, we apply a hydrostatic formula^{23,24} based on the properties of the electron-gas pressure tensor P_{ij} and the Maxwell stress tensor T_{ij}

$$P_{ij} = \frac{2}{5} \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} n(r) \delta_{ij} \quad (2-6)$$

$$T_{ij} = -\frac{1}{4\pi} (E_i E_j - \frac{1}{2} E^2 \delta_{ij}) \quad (2-7)$$

If the electron density $n(r)$ is consistent with the electric field $E(r)$, then

$$\sum_j \frac{\partial P_{ij}}{\partial x_j} = -en(r) E_i(r) \quad (2-8)$$

This is the condition of hydrostatic equilibrium for the electron fluid. The force on an ion immersed in the electron fluid is given by a surface integral:

$$F_i = - \sum_j \int_s (P_{ij} + T_{ij}) dS_j \quad (2-9)$$

The integral is independent of the surface S as long as it surrounds (only) the one ion in question. Eq. (2-6) applies to the Thomas-Fermi groundstate; with a modified definition of ψ_i ; the other formulas extend to finite temperatures or to improved statistical models which include various quantum corrections.²⁴

The electron density $n(r)$ in the colliding ion pair is approximately a superposition of undistorted electron clouds taken from self-consistent calculations for the two separate (isolated) ions:

$$n(\vec{r}) = n_1(|\vec{r} - \vec{R}_1|) + n_2(|\vec{r} - \vec{R}_2|) \quad (2-10)$$

The surface integral is taken over the mid-plane separating the (identical) ions (Fig. 3). With this approximation, the potential $U(R)$ is obtained from a radial (one-dimensional) integration:

$$U(R) = \int_{r=R/2}^{\infty} [g_1(r) \left(\frac{\partial V_1}{\partial r}\right)^2 + A g_2(r) n_1^{5/3}(r)] dr$$

where $n_1(r)$, $V_1(r)$ are the electron density and potential in one (isolated) ion,

$$A = \frac{2}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} 2^{5/3}$$

$$g_1(r) = 2r \left\{ r - \frac{R}{2} - \frac{r^3 - (R/2)^3}{3r^2} \right\}$$

$$g_2(r) = 4\pi r(r - R/2)$$

We can test the superposition approximation for collisions of neutral atoms by comparing with self-consistent solutions given by Lee, Longmire and Rosenbluth.²³ This comparison (Table 2) shows that superposition is very accurate for strong collisions. For weak collisions or large radii, Eq. (2-10) is less accurate.²⁵ For ions, however, the weak collisions are governed by the known asymptotic Coulomb potential.

The screening function $\phi(R)$ is shown in Fig. 4 for several ion charges. The calculations assume $Z_1 = Z_2 = 1$; with scaled radius, the data apply to any collision of similar ions. The plots extend over the range of separations $0 < R < 2R(Z, Q)$. In the superposition approximation, $\phi(R)$ is exactly $Q_1 Q_2 / Z_1 Z_2$ at larger radii.

Fig. 3 Geometry for collision of similar ions with integration plane S bisecting the internuclear axis.

Fig. 4 Numerically calculated screening function $\phi(r)$ for ion-ion interactions as calculated with the superposition approximation. The radius R is scaled to refer to $Z_1 = Z_2 = 1$. Each curve (labelled by the fractional charge of the separate ion) is discontinued at the radius for which the ions first touch.

Figure 4 shows that $\phi(R)$ remains close to $Q_1 Q_2 / Z_1 Z_2$ even down to about $1/2$ the radius at which the ions first touch. Over this range, the ion potential energy is accurately described as a Coulomb potential $U = Q_1 Q_2 e^2 / R$.

Ion Correlations

Next, we consider the spatial distribution of neighbors of a given ion core. This is a statistical problem of classical point particles at positions $R_j(t)$. The particles interact through a potential, usually assumed to have the form:

$$U_{TOT} = \frac{1}{2} \sum_{ij} U(|\vec{R}_i - \vec{R}_j|)$$

where $U(|\vec{R}_i - \vec{R}_j|)$ is $\sim Q^2 e^2 / |\vec{R}_i - \vec{R}_j|$.

A complete analysis of ion dynamics would require examination of many issues, including: 1) the potential energy does not rigorously separate into a sum of additive pairwise interactions; 2) the ion interactions are screened by free electrons,²⁶ which do not necessarily have the same temperature as the ions²; 3) the ion charges fluctuate dynamically due to ionization and recombination²; and, 4) the ion core-repulsion deviates from the Coulomb form at small distances, as shown in Fig. 4.

For Coulomb interactions, the thermal equilibrium ion configurational partition function is:

$$Z_c = \int \frac{d^3 R_1}{V} \int \frac{d^3 R_2}{V} \dots \int \frac{d^3 R_N}{V} \exp \left(-\frac{1}{2} \sum_{ij} \frac{Q_i^2 e^2}{R_{ij} kT} \right) \quad (2-11)$$

and the probability of any specific configuration $\{\vec{R}_j\}$ is

$$\frac{1}{Z_c} \exp \left(-\frac{1}{2} \sum_{ij} \frac{Q_i^2 e^2}{R_{ij} kT} \right)$$

Averages over ion configurations can be evaluated by a Monte Carlo sampling technique introduced by Brush, Sahlin and Teller.²⁶⁻²⁸ The thermodynamic averages depend upon a single parameter

$$\Gamma \equiv \frac{Q^2 e^2}{R_0 kT} \quad (2-12)$$

where

$$R_0 = (3/4\pi n_I)^{1/3} \quad (2-13)$$

is the ion-sphere radius. The ion coupling parameter Γ is the ratio of the Landau length $Q^2 e^2 / kT$ (= distance of closest approach of two ions having kinetic energy kT) to the actual average separation of neighbor ions r_0 . If $\Gamma \ll 1$, the ions move freely in a large volume before colliding with another ion. If $\Gamma > 1$, the ions are being forced together against their Coulomb repulsions; at high Γ the ions are forced into a tightly correlated arrangement which minimizes their electrical energy.

The ion pair-correlation function $g(r)$ is defined such that $n_I g(r)$ is the average density of ions a distance r away from one given ion. With this definition, $g(0) = 0$ and $g(r) \rightarrow 1$ as $r \rightarrow \infty$. In terms of $g(r)$, the static structure factor $S(k)$ is

$$S(k) \equiv 1 + n_I \int g(r) e^{-ik \cdot r} d^3 r \quad (2-14)$$

$g(r)$ or $S(k)$ give a summary description of the average local distribution of neighbors. These functions are spherically symmetric averages and do not retain any information about fluctuating anisotropies in the plasma environment.

A more delicate measure of the local environment is given by the probability distribution $P(E)$ for the electric microfield produced by nearby ions and electrons.¹⁰ This field distribution is used in calculations of line-broadening produced by the Stark effect, a useful plasma spectroscopic diagnostic.⁶⁻¹²

At low densities, the ion correlation is described by Debye-Hückel theory. The ion Debye length D_I is

$$D_I = \left(\frac{kT}{4\pi n_I e^2} \right)^{1/2} = (3\Gamma)^{-1/2} R_0 \quad (2-15)$$

and the number of ions in a Debye sphere

$$\mathcal{N} = \frac{4\pi}{3} n_I D_I^3 = (3\Gamma)^{-3/2} \quad (2-16)$$

The Debye-Hückel theory is a good approximation when $\Gamma \ll 1$, so that $D_I \gg R_0$ and $\mathcal{N} \gg 1$. In this limit, the ion pair-correlation function $g(R)$ and structure factor $S(k)$ are:

$$g(r) = 1 - \frac{Q^2 e^2}{rkT} e^{-r/D_I} \quad (2-17)$$

$$S(k) = k^2 D_I^2 / (1 + k^2 D_I^2) \quad (2-18)$$

In the Debye-Hückel approximation the average potential around a test ion is $V(r) = (Qe/r) \exp(-r/D_I)$. (The potential is modified by additional electron screening.)

The high density limit ($\Gamma \gg 1$) is often described by an ion-sphere picture.^{2,3,27-31} In the simplest version of this model, one assumes

$$g(r) = \begin{cases} 0 & r < R_0 \\ 1 & r \geq R_0 \end{cases}$$

that is, no ion penetrates closer than a distance R_0 . Assuming the free electrons are spatially uniform, this leads to a model potential

$$V(r) = \frac{Qe}{r} + \frac{1}{2} \left(\frac{Qe}{R_0} \right)^2 r^2 - \frac{3}{2} \frac{Qe}{R_0} \quad (2-19)$$

Properly used, the ion-sphere model can give reasonable results for dense plasmas;^{28,30} however, the assumed pair-correlation function is not much like the correct high- Γ form (see Fig. 5).

For dense plasmas, $g(r)$ and $S(k)$ are calculated numerically by Monte Carlo or molecular-dynamics methods. A typical result is shown in Fig. 5. (This case corresponds to $\Gamma = 100$.) The salient features are: few ions at small separations, a ring of nearest neighbors at distance $\sim 1.7 R_0$, and the less sharply defined rings of more distant neighbors.

Molecular Dynamics (MD) simulations integrate classical equations of motion for ion coordinates and give additional information concerning the time-dependence of ion correlations or the dynamic structure $S(k, \omega)$. Recent analytic and numerical results are reviewed by Baus and Hansen.²⁸ Hansen and McDonald³² simulate the complete electron-ion plasma for strong coupling ($\Gamma = 2$) by molecular dynamics. The tendency of classical point electrons to recombine in the attractive $1/r$ potential is inhibited by use of a pseudopotential.³³

Another approach for the static correlation functions is the method of integral equations. Recent applications to the Coulomb system are described by Baus and Hansen,²⁸ and DeWitt and Rosenfield.³⁴

Fig. 5 Ion pair distribution function $g(r)$ for the one component plasma ($\Gamma = 30$) (data supplied by Dr. H. DeWitt). Dashed line indicates the ion-sphere approximation.

A wide range of density-temperature conditions occur in laser-produced plasmas (Fig. 1). In low-density plasma directly heated by the laser, Γ is usually < 1 . DT fuel is also normally in a weak-coupling state ($\Gamma < 1$) because of the small nuclear charge. The ablation plasma, however, often reaches high densities corresponding to $\Gamma = 1$ to 50.

3. FREE ELECTRON COLLISION PHENOMENA

We next consider scattering of free electrons by the ion cores. In conventional plasmas this is simply Rutherford scattering produced by the Coulomb potential Qe/r . However, in dense plasmas the scattering is more sensitive to ion-core structure and to the spatial arrangement of nearby ions.

A simple geometric estimate shows why core structure is more important in dense plasmas: the ion cores occupy a larger frac-

tion of the total volume, as measured by the ratio $(R(Z,Q)/R_0)^3$. A more detailed analysis² shows that the fraction of classical electron orbits which intersect the ion core, i.e., reach the region $r < R(Z,Q)$, is

$$f \approx \frac{1}{3} \frac{\Gamma^2 k T}{Q^2 I} \approx \frac{1}{3} \frac{\Gamma}{Q} \frac{R(Z,Q)}{R_0}$$

In a low-density plasma, $f \ll 1$, and most collisions involve only the asymptotic Coulomb potential. In a dense plasma, f may approach unity, and calculation of the electron mean free path requires detailed information about ion core positions and potentials.

Consider an electron interacting with an assembly of many ions. To the accuracy of the superposition approximation (see Eq. (2-10) and Table 2), the total electrostatic potential is a superposition of contributions from the individual ions:

$$V(\vec{r}) = \sum_j V(\vec{r} - \vec{R}_j) \quad (3-1)$$

The ion cores are assumed to be located at fixed positions $\vec{R}_j$ during the scattering. The individual ion potential $V(\vec{r} - \vec{R}_j)$ is determined by some model for ion-core structure such as the Thomas-Fermi theory.

When a free electron scatters from the assembly of ions, the scattered waves interfere. In the Born approximation, the resulting cross-section per ion, in differential form, is

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{isolated ion}} S(q)$$

where

$\hbar k = mv$ = initial (electron) momentum

$\hbar q = 2mv \sin \theta/2$ = momentum transferred

$V(q)$ = Fourier transform of one-ion potential

$S(q)$ = plasma structure factor, defined in Eq. (2-14)

The momentum transport cross-section, $\sigma_{tr} = \int (1 - \cos \theta) d\sigma/d\Omega d\Omega$, is then

$$\sigma_{tr} = \frac{\pi}{k^4} \left(\frac{em}{2\pi\hbar^2} \right)^2 \int_0^{2k} q^3 |V(q)|^2 S(q) dq \quad (3-2)$$

In condensed-matter physics, Eq. (3-2) is often called the Ziman formula. The interpretation is that small-angle scattering is limited by interference of scattered waves originating on neighbor ions. The structure-factor $S(q)$ operates as a form-factor describing the spatial distribution of neighbor ions.

Equation (3-2) can be evaluated analytically in the Debye-Hückel limit. For fully stripped ions, the potential $v(q)$ is simply:

$$v(q) = 4\pi q e / q^2$$

The structure factor $S(q)$ is given in Eq. (2-18). With these approximations, the electron mean-free-path is:

$$\frac{1}{\bar{\ell}} = n_I \sigma_{tr} = \frac{4\pi Q^2 e^4 n_I}{m^2 v^4} \left[\frac{1}{2} \ln \left(1 + \frac{4m^2 v_D^2}{\hbar^2} \right) \right] \quad (3-3)$$

This is the usual result of multiple-scattering theory for the Lorentz gas. The logarithmic factor is called the Coulomb logarithm.

It is reassuring that the Ziman formula reduces to the usual cross-section for low-density fully-ionized plasmas, but inertial fusion applications will require data for dense and partially-ionized material. At high densities, the structure factor $S(q)$ is the Fourier transform of a strongly-peaked pair-distribution $g(r)$ [see Fig. 5]. Information about the ion core enters Eq. (3-2) through the potential $V(q)$, which deviates from the pure-Coulomb form for partially-stripped ions. Together, these two corrections dramatically change the mean free path at high-density conditions.

Eq. (3-2) can be evaluated by combining numerical structure-factors $S(q)$ from the one-component plasma together with electron-ion potentials $v(r)$ obtained from a self-consistent field method. This recipe is not completely satisfactory because the Born approximation is inaccurate when applied to low-energy electrons. One can improve Eq. (3-2) by replacing the matrix-element $V(q)$ of the potential by a T-matrix element $T(k, q)$ calculated by partial-wave scattering theory.³⁵

A comprehensive study of the transport coefficients for degenerate low-Z dense plasmas (appropriate to white-dwarf interiors) is given by Minoo, Deutsch and Hansen.³⁶ These authors survey the earlier astrophysical literature and compare several approximations. More recent calculations aimed at the range $\Gamma \leq 1$ are given by Boercker, Rogers and DeWitt. This work,³⁷ and the interesting work of Hansen, et al. concentrate on exploring a

dynamical screening theory including frequency-dependent structure factors $S(k, \omega)$ and electron-ion correlations.

A practical formula for high-density thermal conductivity is given by Brysk, et al.³⁸ Brysk's approach was recently extended to provide a comprehensive package of transport coefficients (including thermoelectric and thermomagnetic effects) which are approximately valid for arbitrary plasma conditions and composition.³⁹

So far, the discussion considers only elastic scattering of electrons by ions. We are also interested in density effects on inelastic cross-sections. Preliminary investigations indicate that plasma screening changes the cross-sections for inelastic processes involving small energy-transfers.⁴⁰

Conduction Inhibition

Electron thermal conduction is very important to the establishment of an ablation flow profile in laser-target interaction (see Fig. 1). However, the temperature gradient at high laser intensities is as large as

$$\frac{\partial T}{\partial x} \sim \frac{1 \text{ keV}}{10 \mu} \sim 10^{10} \text{ }^\circ\text{K/cm}$$

and in this circumstance it is no surprise that the usual linear transport theory is inadequate. The expansion in powers of $\partial T / \partial x$ has failed.

Theoretical expectations based on kinetic theory suggest that the heat current density would saturate at a maximum

$$q_{\text{max}} \approx f n_e kT \sqrt{\frac{kT}{m}}$$

where $f \approx 0.6$ follows from a Knudsen gas model. Experiments do not support this expectation; a large number of spherical and planar laser irradiation experiments are empirically replicated by simulations in which the heat current is strongly inhibited to values corresponding to $f \sim 0.05$. The heat flow inhibition is probably the most important unexplained phenomenon observed in laser-target interactions.⁴¹

Recently, it has been realized that the majority of the heat current is carried by energetic electrons ($E \geq 10 \text{ kT}$) in the tail of the thermal distribution. In an ablation plasma, collisional ionization removes these electrons; it may remove them so rapidly that they cannot be replaced by electron-electron collisions. In this way, atomic ionization may contribute significantly

to conduction inhibition along with other mechanisms which distort the electron distribution function.⁴²

4. ELECTRON STATES I

For a more detailed analysis of dense-plasma processes, it is necessary to calculate atomic properties such as electron energy spectra, line-strengths and electron-impact cross-sections. This data is needed for an arbitrary atom in a plasma of arbitrary density and temperature. It is natural to attack this problem by extending the usual self-consistent field method. Using this approach, Liberman⁴³ considers a single nucleus centered in a spherical cavity in a positive charge background. The electron energies ϵ_s and wave-functions $\psi_s(r)$ are found by solving the one-electron Schroedinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_s + [V(r) + V_{xc}(r)] \psi_s = \epsilon_s \psi_s(r) \quad (4-1)$$

It is usual to include an exchange or local-density exchange-correlation potential V_{xc} . (Liberman solves the Dirac equation and uses the zero-temperature Kohn-Sham exchange potential.)

For thermal equilibrium (LTE) plasmas, each electron state is independently occupied according to Fermi-Dirac statistics,

$$f_s = [1 + \exp(\epsilon_s - \mu)/kT]^{-1} \quad (4-2)$$

From this assumption, it follows that the average electron density is

$$n(r) = \sum_s f_s |\psi_s(r)|^2 \quad (4-3)$$

This electron density is required to be consistent with the original potential $V(r)$.

At first sight this may appear to be a reasonably rigorous approach, but the reader will notice that Eq. (4-2) implies that electron states are occupied by fractional numbers of electrons. The calculation yields one-electron eigenvalues representing the spectrum of the so-called average atom. Electron eigenvalues are averaged over ionization and excitation states of the central ion, as well as the entire local plasma environment. The average eigenvalues $\epsilon_s = \epsilon_s(\rho, T)$ depend on density and temperature primarily because of shifts in the dominant ionization stage $Q(\rho, T)$.

Assuming we adopt the average-atom viewpoint, many interesting questions of detail arise. Liberman explores two alternative formulations of the cavity model which differ in the way atomic properties are distinguished from those of the background. Choices must be made for the manner in which neutrality is enforced, for the pressure formula, and for boundary conditions imposed on the wavefunctions.

Alternative versions of the spherical-cell model are described by Perrot,⁴⁴ Berggren and Froman,⁴⁵ Rozsnyai⁴⁶ and others.^{40,47}

Bound electrons have energy less than the asymptotic potential, which may be taken to be zero; outside the cavity, bound-state wavefunctions decrease exponentially with radius. Because of the spherical symmetry of the potential, the eigenvalue $E_{n,l,j}$ has degeneracy $2j + 1$.

At positive energies, there are continuum states composed of an incident plane wave scattered into various angular-momentum channels. Resonance scattering is produced by the centrifugal barrier surrounding the inner electrostatic well. Scattering resonances contribute peaks to the continuum density of states; in a nonrelativistic theory,

$$g(\epsilon) = c_1 \sqrt{\epsilon} + \frac{2}{\pi} \sum_l (2l+1) \frac{d\delta_l}{d\epsilon}$$

and a narrow resonance gives a sharply-defined peak. Early cell-model calculations neglected the resonance contribution and consequently predicted unphysical discontinuities during pressure ionization.

It is useful to develop a simple representation of the one-electron energy-levels emerging from self-consistent field calculations. For non-relativistic spectra, a WKB approximation gives:

$$E_{n,l} = E_n^0 - \frac{Q_n^2 e^2}{2a_0 (n - \Delta_{nl})^2} \quad (4-4)$$

$$r_n = a_0 n^2 / Q_n \quad (4-5)$$

r_n is the classical (Bohr) orbit radius, determined as the harmonic average over a WKB wave-function, i.e., $1/r_n = \langle n, l | 1/r | n, l \rangle$. Defining a screening function $Z(r)$ from the atomic potential by $V(r) = Z(r)e/r$, we have

$$Q_n = \left[Z(r) - r \frac{dZ}{dr} \right]_{r=r_n} \quad (4-6)$$

$$E_n^0 = -e^2 \left[\frac{dZ}{dr} \right]_{r_n} \quad (4-7)$$

where Q_n is the charge corresponding to the electric field at radius r_n and $\Delta_{n,l}$ is a quantum defect. For high quantum numbers (Rydberg states), $\Delta_{n,l}$ is approximately independent of n and is associated with the inner turning point of the classical orbit. For inner-shell electrons, $\Delta_{n,l}$ has contributions from both inner and outer turning points. The screened charge Q_n and quantum defect $\Delta_{n,l}$ depend on plasma density and temperature.

More elaborate screening models are discussed by Rogers⁴⁸ and Huebner⁴⁹. Huebner shows that photoelectric cross-sections are governed by the inner-screening charge Q_n (rather than the effective charge $Z(r_n)$ defined from the potential).

A simpler screening model finds extensive application in fusion research (Mayer,⁵⁰ Post et al.,⁵¹ Lokke and Grasberger⁵²). The screened hydrogenic model is obtained from Eq. (4-4) if one neglects the quantum defects:

$$E_{nl} + E_n = E_n^0 - \frac{Q_n^2 e^2}{2a_0 n^2} \quad (4-8)$$

$$r_n = a_0 n^2 / Q_n \quad (4-9)$$

The screened charges Q_n are calculated as linear combinations of the shell populations (now simply functions of the principle quantum number n):

$$Q_n = Z - \sum_m \sigma(n,m) P_m \quad (4-10)$$

The screening coefficients $\sigma(n,m)$ represent the overlap of wavefunctions of n th and m th shells. Mayer⁵⁰ gives screening coefficients based on perturbation theory for hydrogenic atoms; an alternative set⁵ gives more accurate ionization potentials for nearly-neutral atoms.

Eq. (4-8) describes a Bohr atom with effective charges. The electrostatic potential at radius r_n consists of the potential

outside a core of charge $Q_n e$ plus a sum of potentials inside shells having charge $-e P_m$ located at radii $r_m > r_n$:

$$V(r_n) = \frac{Q_n e}{r_n} - \sum_{m>n} \frac{P_m e}{r_m} \sigma(m, n) \quad (4-11)$$

The electron orbits are quantized by the Bohr formulas:

$$m v_n^2 / r_n = Q_n e^2 / r_n^2 \quad (4-12)$$

$$m r_n v_n = n \hbar \quad (4-13)$$

these assumptions give energies

$$E_n = \frac{1}{2} m v_n^2 - e V(r_n) = - \frac{Q_n^2 e^2}{2 a_0 n^2} + E_n^0 \quad (4-14)$$

in agreement with Eq. (4-8). The electron-electron energy is evaluated using the harmonic-mean property of r_n ; the result is a simple expression for the total ion energy $E_{TOT} = \sum_n E_n P_n - U_{ee}$:

$$E_{TOT} = \sum_n \left(- \frac{Q_n^2 e^2}{2 a_0 n^2} \right) P_n \quad (4-15)$$

The eigenvalue E_n is the derivative of E_{TOT} with respect to the population P_n ; i.e., if Eq. (4-15) is regarded as an effective or model Hamiltonian, it satisfies Koopman's theorem with the eigenvalue E_n of Eq. (4-14). This property is required for thermodynamic consistency.

For thermal equilibrium applications of the average-atom model, the integer population P_n is replaced by an average population calculated from Fermi statistics,

$$\bar{P}_n = \frac{D_n}{1 + \exp(E_n - \mu)/kT} \quad (4-16)$$

where $D_n = 2n^2$ is the shell degeneracy. The energy E_n appearing in (4-16) is obtained by consistently solving Eqs. (4-10, -11, -14) with the average populations $\bar{P}_n$. This is essentially the finite-temperature Hartree approximation for the model Hamiltonian (4-15).

Average-atom eigenvalues depend strongly on temperature: as temperature rises, bound electrons are thermally ionized and the screened charges Q_n increase. As a result, the energy-levels increase with temperature, so that spectral lines shift toward higher energies. For the quantum self-consistent field theories (Eqs. 4-1 to 4-3), the ℓ -splitting of levels decreases as the hydrogenic limit is approached (for high-Z atoms, there is relativistic spin-orbit splitting even in the hydrogenic limit).

The density-dependence of average-atom eigenvalues is much weaker. Numerical results from self-consistent field calculations show that the density-dependence is principally caused by recombination which reduces the effective charges Q_n .

Smaller contributions are produced by two other density effects. First, at higher density there is a higher degree of thermal excitation, and this excitation alters the self-consistent potential, in turn producing a shift of energy levels. Second, a small shift is associated with inner screening of bound electrons by free electrons, often called the plasma polarization shift. Both effects are too small to be easily resolved in average-atom self-consistent field calculations.

Pressure Ionization and Density Effects on Outer Electrons

Electron states with large quantum numbers are obviously very sensitive to events in the surrounding plasma.

These states are important in three ways: first, the atomic partition function would diverge if states with high quantum-number were included; second, the highly-excited bound states are important for line absorption and dielectronic recombination; third, at high density, the plasma begins to perturb occupied core levels important to the thermodynamic energy of the plasma.

Many authors calculate energy-levels, collision cross-sections, and oscillator-strengths for a Debye-screened atomic potential. However, there are objections to this model even at low densities ($\Gamma \ll 1$) where the Debye-Hückel theory is valid.⁵ The basis of these objections is that, for large radii ($r > R_0$), the Debye potential is the small average of a large fluctuating field. A bound electron having large orbit radius $r_n > R_0$ has low velocity $v_n \sim Q_n e^2 / \hbar n$ and responds much more strongly to the fluctuations than to the small average potential.* For example, the mean free

*It may clarify this situation to point out that when $\Gamma \gg 1$, the Debye theory correctly gives the average potential and also the average of any linear function of $V(r)$, such as the plasma coupling energy. The Debye potential is not satisfactory when used to describe quantities (such as boundstate eigenvalues) which depend on the potential in a nonlinear way.

path of a Rydberg electron is less than the orbit circumference whenever as $r_n > R_0$.

Quantum cell calculations based on Eqs. (4-1, 2, 3), show that electron eigenstates are forced into the continuum at densities where the ion-sphere radius R_0 becomes less than the orbit radius $r_n = a_0 n^2 / Q_n$. This simple geometric criterion is algebraically equivalent to an energetic criterion which compares the binding energy $-Q_n^2 e^2 / 2 a_0 n^2$ to the potential $-Q e^2 / R_0$ by which the neighboring lower the continuum edge.²

A practical model for pressure ionization can readily be constructed for the average-atom model.⁴ In this picture, boundstates become continuum resonances as soon as they move to positive energy. The resonance states are no longer completely orthogonal to continuum wave-functions, especially for broad resonances.⁵³ In practice, this transition is modelled by reducing the shell degeneracy D_n from $2n^2$ to zero as the atom is compressed past the critical radius $R_0 = r_n$.

The remainder of the state density $(2n^2 - D_n)$ appears in the lowered continuum. Because fractional populations are essential to this method (D_n is a smooth function of density), it applies to the average-atom model but would not make sense for the original Saha theory.

This pressure-ionization model suffices for description of light atoms but is not very satisfactory for transition metals or heavier atoms. A more detailed electronic energy spectrum, including subshell splitting, is required to calculate thermodynamic properties of high-Z plasmas.

5. ELECTRON STATES II

The average-atom model (AA) is heavily used in practical calculations for both magnetic and inertial fusion, whether in the quantum cell-model formulation of Eqs. (4-1, 4-3) or in the algebraic screened hydrogenic model of Eqs. (4-8) to (4-15).

For low-Z or nearly-ionized atoms, detailed atomic energy-levels are known, and most scientists prefer to work in this representation (often called detailed configuration accounting or DCA method). It is useful to compare the AA and DCA pictures in order to identify essential limitations of the AA description.

Few-Electron Ions

We first consider a low density, low-Z plasma which contains ions in hydrogen-like and helium-like ionization stages.

In hydrogen-like ions, $1s \rightarrow 2p$ transitions have an energy

$$h\nu = (Z^2 - \frac{1}{4} Z^2) e^2/2a_0 \quad (5-1a)$$

The helium-like ions have a corresponding transition $1s^2 \rightarrow 1s2p$ at an energy near

$$h\nu = [(Z - 0.66)^2 - (Z - 1)^2/4] e^2/2a_0 \quad (5-1b)$$

The average-atom model gives instead a single $1s \rightarrow 2p$ absorption line at an average energy determined by the relative number of hydrogenic and helium-like ions in the plasma. If the energy of this transition is calculated from the Mayer screening model (using the initial populations),

$$h\nu_{AA} = [(Z - 2\sigma_{11}P_1)^2 - \frac{1}{4} (Z - \sigma_{21}P_1)^2] e^2/2a_0 \quad (5-1c)$$

This is equivalent to an average of Eqs. (5-1a, b) except for (1) possible minor differences in the screening constants, and (2) a difference between $\langle P_1 \rangle^2$ and $\langle P_1^2 \rangle$, i.e., nonlinearity in the average.

The cross section for line absorption with excitation of a $1s$ electron to a $2p$ state is

$$\sigma_{abs} = P_{1s} (D_{2p} - P_{2p}) \frac{\pi e^2}{mc} f_{1s \rightarrow 2p} \quad (5-2)$$

where $f_{1s \rightarrow 2p}$ = average oscillator strength, and $D_{2p} = 6$ = final state degeneracy. Equation (5-2) applies in a detailed configuration description, where the populations are integers, and must be averaged over ions. The average-atom model calculates the absorption cross-section from the same equation, with $\langle P_{1s} (D_{2p} - P_{2p}) \rangle$ replaced by $\langle P_{1s} \rangle (D_{2p} - \langle P_{2p} \rangle)$; this is understood to give the total cross-section for transitions $1s \rightarrow 2p$ for any ion.

Although the average photon energy (5-1c) and average absorption cross-section are reasonable, it is dangerous to replace two absorption lines by one stronger line in a calculation of line-transport or line-formation.

In certain cases, the averaged version of Eq. (5-2) is very misleading. For example, consider a plasma consisting of H-like, He-like and Li-like groundstate ions. The existence of hydrogen-like ions implies $\langle P_{1s} \rangle < 2$ and the presence of Li-like ions implies $\langle P_{2s} \rangle > 0$. If each ion is in its groundstate, the actual emission rate is zero.

In the average-atom description of this plasma, $\langle P_{2s} \rangle \neq 0$ and $\langle P_{1s} \rangle < 2$ and so the average atom emits radiation (with the aid of Stark splittings which break the usual selection rules).³¹ In this case, the AA prediction is totally incorrect, a failure which may be traced to the assumption $\langle P_{2s}(D_{1s} - P_{1s}) \rangle = \langle P_{2s} \rangle (D_{1s} - \langle P_{1s} \rangle)$.

In dense plasmas, there are excited H-like, He-like ions present together with the Li-like ions. In this case the average-atom rates are closer to correct.

From the limited information given by the average populations, it is not possible to work backward to the individual ion densities, unless an additional assumption (such as LTE) is added.

Another interesting problem arises for ions with metastable levels such as the $1s2p$ triplet state of helium. The DCA description is able to distinguish between $1s2p$ singlet and triplet populations, but the average-atom model has no degree of freedom to describe this difference. Rate equations for the average atom predict that an isolated excited atom will decay to its groundstate without any vestige of metastability.

In a dense plasma collisions may break up metastable states and electric fields may be large enough to enable forbidden transitions (such as $2s \rightarrow 1s$). Nevertheless we must be very cautious in using the results of average-atom calculations.

Complex Atomic Spectra

When the spectrum becomes complex with many thermally excited electrons, the number of configurations rises dramatically. Under these conditions, it is impractical to accurately calculate all the energy levels and oscillator-strengths for transitions between them. In this case the average-atom description is attractive because of its computational simplicity. The question is whether it affords an accurate description of the atomic statistical problem. This question has been addressed in the context of LTE plasmas by Mayer,⁵⁰ Green,⁵⁴ Grimaldi and Grimaldi-Lecourt⁵⁵ and More.²

Let us consider a comparatively heavy atom (niobium) in thermal equilibrium at 200 eV. We will compare AA and DCA calculations for the atomic spectrum generated by Eqs. (4-8 to 14).²

In the DCA, atomic states are characterized by the populations of various shells: a group of states is labelled by integer populations P_n where $0 < P_n < 2n^2$. The ion charge is $Z^* = Z - \sum_n P_n$ and the effective charges (defined by Eq. 4-10) are

$Q_n = Z - \sum_m (n, m) P_m$. The ion energy is determined by the approximate Hamiltonian of Eq. (4-15):

$$E_{TOT} = - \sum_n \left(\frac{Q_n^2 e^2}{2a_0 n^2} \right) P_n$$

The group of states so described is highly degenerate. The number of quantum states is

$$C = \prod_n \frac{D_n!}{P_n! (D_n - P_n)!}$$

These states are generated by permutations of the electrons over allowed single-particle states consistent with the stipulated shell populations $\{P_n\}$.

The probability of the set of populations $\{P_n\}$ is, for a thermal equilibrium plasma,

$$P(\{P_n\}) = \frac{N}{C} \exp \left(- \frac{E_{TOT} + F_0}{kT} \right)$$

where C = combinatorial factor, F_0 = free energy of Z^* free electrons in the average atomic volume V , and N = normalization factor (reciprocal of the partition function). With this probability distribution, we calculate average populations $\langle P_n \rangle$ and other averages. A typical calculation requires summation over 10^5 sets of populations $\{P_n\}$:

Some conclusions which emerge from this study are:

- 1) The averages of P_n are within 10% of values calculated using Fermi functions as in Eq. (4-16).
- 2) The number of thermally excited configurations rises very rapidly with plasma density so that the average of C is $\sim 10^{10}$ for Nb at 200 eV, 1 g/cc.

Fig. 6 Average atomic excitation energy (relative to groundstate ions) for an LTE niobium plasma as calculated by the detailed configuration method.

- 3) The internal excitation energy rises rapidly with density for atoms having many bound electrons (Figure 6).

The summation over all sets of populations includes states with arbitrarily inverted populations (e.g., vacancies in k-shell) and thus includes many autoionizing states. It is found that the average excitation energy is large enough, for Nb at 200 eV and 1 g/cc, to allow many (3-5) autoionizations.

Elaborate analytic investigations of the corrections to average-atom populations are reported by Green⁵⁴ and Grimaldi and Grimaldi-Lecourt.⁵⁵

6. NONEQUILIBRIUM PLASMA STATES

Calculations of non-equilibrium atomic processes are often performed using a non-LTE version of the screened hydrogenic average-atom model described in section 4. The equilibrium equation for average shell populations, Eq. (4-16), is replaced by a rate equation including transitions caused by collisional and radiative mechanisms. Details of this model are described in the lecture of G. Zimmerman,⁵⁶ and in various other reports.^{1,2,51,52}

The non-LTE average-atom model is subject to the list of critical comments given in section 5. In addition, we note that (1) hydrogenic rate coefficients and oscillator-strengths are not very accurate; (2) the usual model does not include possible density effects on cross-sections; and (3) it is always assumed that the majority of free electrons have an equilibrium (Maxwellian or Fermi-Dirac) distribution.⁴²

Laser-produced plasmas depart from thermal equilibrium in many ways, and there is a natural temptation to develop increasingly comprehensive kinetic models, which allow numerical treatment of an arbitrary nonequilibrium states. This approach may be the best method to improve the fundamental accuracy of our physical modelling, but there is also a role for approximate treatments which bring out the physical character of realistic but simplified modes of departure from thermal equilibrium. Results of this second type have the advantage of suggesting intuitive ideas that we can work with.

Non-LTE Electron Populations

Because of the relevance to astrophysical and low-density laboratory plasmas, there is a great deal of literature analyzing the steady coronal or collisional-radiative plasma.^{9,12,31,51,52,57} In this model, an atom is coupled to Maxwellian free electrons at a fixed temperature T_e and allowed to radiate freely (i.e., coupled to a radiation field at $T_R = 0$). Salzmann⁵⁸ formulates the CR model in an interesting way which emphasizes the density-dependence of bound-electron populations in optically-thin matter.

High-density plasmas of ICF interest are often not optically thin, and a coronal or collisional-radiative model is too extreme a simplification. A greater degree of realism is provided by a model in which the radiation field has a black-body distribution at a temperature somewhat lower than T_e . We therefore consider an atom coupled collisionally to free electrons having a high temperature T_e and coupled radiatively to a black-body distribution at a lower temperature T_R .

To greatly simplify the formulas, consider a two-level atom which has eigenstates $1>$ and $2>$. P_1 and P_2 denote the populations of each state ($P_1 + P_2 = 1$). [The final result is more general than implied by this simple model.] The populations evolve due to collisionally induced transitions:

$$\left(\frac{dP_1}{dt}\right)_e = -aP_1 + a e^{E/kT_e} P_2 \quad (6-1)$$

and radiatively induced transitions

$$\left(\frac{dP_1}{dt}\right)_R = -bP_1N_V + bP_2(N_V + 1) \quad (6-2)$$

where $E = h\nu$ = energy difference between the levels, and N_V = number of photons per mode $= \left(e^{h\nu/kT_R} - 1\right)^{-1}$. The notation can be simplified by defining

$$\frac{\gamma}{a} = bN_V \quad \frac{\gamma}{a} e^{E/kT_R} = b(N_V + 1)$$

so that

$$\left(\frac{dP_1}{dt}\right)_R = -\frac{\gamma}{a} P_1 + \frac{\gamma}{a} e^{E/kT_R} P_2 \quad (6-3)$$

For the equations given, only photons of frequency $h\nu$ are coupled to the atom; in a more realistic treatment the atom is coupled to photons of arbitrary frequencies via photoelectric processes.

The steady-state populations are determined by requiring the time-derivative P_1 to vanish. This is a linear equation for P_1 whose solution is:

$$P_1 = \frac{\frac{\gamma}{a} e^{E/kT_e} + \frac{\gamma}{a} e^{E/kT_R}}{\frac{\gamma}{a} (1 + e^{E/kT_e}) + \frac{\gamma}{a} (1 + e^{E/kT_R})} \quad (6-4)$$

Entropy is produced in three ways in the system considered. If the atomic populations change, then the atomic entropy production is

$$\dot{S}_{\text{atom}} = -k P_1 \log (P_1/P_2) \quad (6-5a)$$

Entropy produced in the heat baths is given by

$$\dot{S}_e = \frac{h\nu}{T_e} \left(\frac{dP_1}{dt}\right)_e \quad (6-5b)$$

$$\dot{S}_R = \frac{h\nu}{T_R} \left(\frac{dP_1}{dt}\right)_R \quad (6-5c)$$

If the time-derivatives are eliminated via Eqs. (6-1, 6-3), then the rate of entropy production is expressed as a function of the atomic population P_1 .

We can vary the population P_1 to determine the state of minimum rate of entropy production. In general, the resulting state is not identical to the steady-state determined in Eq. (6-4). However, in the special case $|T_R - T_e| \ll T_e$ where the system is close to equilibrium, it turns out that the state of minimum entropy production is identical, to first order in $\Delta T = |T_R - T_e|$ to the steady-state given by Eq. (6-4).

Therefore, principle of minimum entropy production characterizes the steady nonequilibrium state to first order in the departure from complete thermal equilibrium.^{59,60}

In qualitative terms, one can say that the atomic system occupies the state which minimizes the steady-state rate of conversion of electron energy into radiation. This statement is not an exact paraphrase of the result established because the conversion efficiency is actually the rate of energy transfer, not quite identical to the rate of entropy production. In real laser-interaction plasmas, there are additional physical complexities which change the situation, including effects of spatial gradients, transient or dynamic effects, and departures from the limit $\Delta T \ll T$.

Within the linear regime ($\Delta T \ll T$), we have found that the minimum entropy production principle also characterizes the steady state of more complicated models including the complete non-LTE average atom model described above.

Electron-Ion Nonequilibrium

Several plasma processes induce an electron-ion temperature difference:

- 1) Laser radiation heats the free electrons,
- 2) Free electrons cool by emission of bremsstrahlung and recombination radiation, and
- 3) Ions are heated by strong shock-waves or by adiabatic compression in an implosion.

Electron-ion heat transfer is strongly impeded by the inequality of electron and ion masses. Estimates of collisional heat exchange show that the time to equilibrate electron and ion temperatures often exceeds laser deposition or plasma flow time-scales.

If the plasma density is low, it is reasonable to assume a two-fluid model of interpenetrating ideal gases having separate temperatures (T_e, T_i) and additive properties. In dense plasmas, the Coulomb interactions are strong enough to significant-

ly modify the ideal-gas equation of state and a better description is needed.

We consider a nonequilibrium steady plasma characterized by unequal electron and ion temperatures. The screened ion pair-potential in such a two-temperature plasma may be taken as

$$U(R) = \frac{Q_1 Q_2 e^2}{R} \exp\left(-\frac{R}{D_e}\right) \quad (6-6)$$

where $D_e = D_e(T_e)$ is the Debye-length associated with electron screening. Any sudden energy-deposition into the electrons raises their temperature and then is communicated to the ions on two separate time-scales:

- 1) Nearly instantaneously (time $\sim 1/\text{electron plasma frequency}$) as an alteration of the screening length D_e , the ion pair-potential $U(R)$ and the subsequent thermal motion of the ions. The Coulomb interactions transfer energy in the form of electrical work between the two species.
- 2) More slowly, through collisions that transfer random thermal energy (heat) from electrons to ions.

A straightforward statistical treatment² shows that pressure, energy, and other variables are functions of electron temperature T_e , ion temperature T_i , and volume V . Changes of the energy $E = E(T_e, T_i, V)$ obey

$$dE = T_e dS_e + T_i dS_i - p dV \quad (6-7)$$

where S_e and S_i are separate entropies associated with the phase space occupied by electron and ion distributions. The pressure and energy do not separate into additive contributions except at low densities.

A generalized condition of thermodynamic consistency is found to be

$$\left(\frac{\partial E}{\partial V}\right)_{T_e, T_i} = T_e \left(\frac{\partial p}{\partial T_e}\right)_{T_i, V} + T_i \left(\frac{\partial p}{\partial T_i}\right)_{T_e, V} - p \quad (6-8)$$

This equation is a constraint on any approximate model for the thermodynamic properties of nonequilibrium plasmas. The partial derivative $\partial p / \partial T_e$ is defined as a derivative for constant volume V and ion temperature T_i ; for the case of thermal equilibrium

($T_e \approx T_I$), Eq. (6-8) reduces to the usual thermodynamic consistency relation.

Practical specific heat coefficients can be defined by

$$dT_e = A_{ee} dQ_e + A_{eI} dQ_I \quad (6-9)$$

$$dT_I = A_{Ie} dQ_e + A_{II} dQ_I \quad (6-10)$$

$dQ_e = T_e dS_e$ = heat added to electrons, $dQ_I = T_I dS_I$ = heat added to ions. These equations apply to an infinitesimal transformation occurring at constant volume V . Through use of a Maxwell relation generated from Eq. (6-7), we can show

$$\frac{A_{eI}}{T_e} = \frac{A_{Ie}}{T_I} \quad (6-11)$$

If an amount of heat dQ_e is suddenly added to the electrons (e.g., by a short laser pulse), then Eqs. (6-9, 10) assert that both electron and ion temperatures will rise. The change in ion temperature is produced indirectly by the sudden reduction in the electron screening which strengthens the potential $U(R)$ and immediately is reflected in the ion kinetic energy.

Equations (6-7) through (6-11) are derived² by assuming a canonical ensemble distribution function for the position and velocity distribution of the ions based on the potential of Eq. (6-6). The Born-Oppenheimer approximation is essential to the derivation.

The two-temperature effects are largest at dense-plasma conditions, where the electron-ion interaction energy is a significant perturbation of the ideal-gas equation of state. Analytic formulas for the electron-ion energy are available only in the low-density limit.

7. DENSE ATOMIC PLASMAS (SUMMARY)

The dense plasma is normally defined as a strongly coupled electron-ion system in which the ion correlation length (Debye length) is so short that the screening is complete within a few atomic spacings. The Coulomb system is essentially classical and forms a background or environment for the atomic physics. The dense atomic plasma has the additional ingredient of partial ionization.

For partially ionized plasmas, the ionization state Q is a self-adjusting quantity. For example, when the electron-ion

interaction, measured by Qe^2/R_0 , becomes large enough to be comparable to kT , free electrons recombine and the interaction is reduced. As shown by Eq. (2-2) the ionization adjusts itself so that $I(Z,Q)$ is a multiple of kT --typically, $\sim 10 kT$ in a low-density LTE plasma, but as little as $\sim 2 kT$ in a dense plasma. In low-density plasmas, the large ratio $I(Z,Q)/kT$ implies a strong energetic decoupling of bound electrons from the free particles of the plasma.

Let us summarize changes which occur when a nondegenerate equilibrium (LTE) plasma is compressed at constant temperature.

As the density rises, the average ion charge state Q decreases. Because of this, the ionization potential of the outermost bound electron falls and the ratio I/kT decreases. The excitation energies are submultiples of the ionization potential, and so the typical excited state is closer to the groundstate in a dense plasma. Because of the reduced energy required for excitation, the average number of excited electrons increases.

In low-density plasmas, electron-ion scattering is controlled by the simple Coulomb potential Qe^2/R for most collisions. Contrawise, in dense plasma, the non-Coulomb core potential is important because the cores fill a large fraction of the plasma volume.

In dense plasma, excited states near the continuum are more often occupied. These states interact strongly with neighbor ions, and can be understood only through more elaborate models than those used for more deeply bound electrons. Collisional ionization and recombination rates greatly increase in dense plasmas (approximately proportional to density squared), so that ionization and bound populations fluctuate on shorter time-scales.

Thus, the atom in a dense plasma has more active degrees of freedom and plays a more vigorous dynamical role than in low-density plasmas. The conclusion emerging from this analysis is very clear: dense plasmas containing partially-stripped ions are very interesting from the atomic point of view.

APPENDIX A.

THE ISOLATED GROUNDSTATE TF ION

The model describes an ion of nuclear charge Z and ion charge Q . The Thomas-Fermi equations are:

$$\nabla^2 V = 4\pi n(r) \quad (A1)$$

$$n(r) = \frac{1}{3\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (\mu + eV(r))^{3/2} \quad (A2)$$

where $V(r)$ = electrostatic potential, e = electron charge, $n(r)$ = electron number density, μ = electron chemical potential. Eq. (A1) expresses electrostatic self-consistency, and Eq. (A2) gives the zero-temperature (i.e., groundstate) electron density of a semiclassical electron gas. The isolated ion is spherically symmetric. The boundary conditions for Eqs. (A1, A2) are:

$$V(r) + \frac{Ze}{r} \rightarrow 0 \quad r \rightarrow 0 \quad (A3)$$

$$V(r) = \frac{Qe}{r} \quad r > R_i \quad (A4)$$

where R_i = radius at which $n(r)$ first equals zero. From Eq. (A2),

$$\mu = -Qe^2/R_i \quad (A5)$$

we also have

$$Z - Q = \int n(r) d^3r \quad (A6)$$

The contributions to the ion's energy are:

- 1) Electron-gas kinetic energy:

$$K = \int \left[\frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2 n(r))^{2/3} \right] n(r) d^3r \quad (A7)$$

- 2) Electrostatic interaction of electrons with nucleus:

$$U_{en} = - \int \frac{Ze^2}{r} n(r) d^3r \quad (A8)$$

3) Electron-electron interaction:

$$U_{ee} = \frac{e^2}{2} \int \frac{n(r) n(r')}{|r - r'|} d^3r d^3r' \quad (A5)$$

Eq. (A9) can easily be reduced to a one-dimensional (radial) integral.

The total ion energy is $E_{TOT} = K + U_{en} + U_{ee}$. There is a variational theorem by which $E_{TOT} = E[n(r)]$ is minimal for the correct electron density $n(r)$, subject to the constraint of Eq. (A6). From Eq. (A2) it follows that:

$$\mu(Z - Q) = \frac{5}{3} K + U_{en} + 2U_{ee} \quad (A10)$$

The virial theorem yields the relation

$$2K + U_{en} + U_{ee} = 0 \quad (A11)$$

The virial theorem is a consequence of Eq. (A1, A2) and not an additional assumption. Equations (A10, A11) give

$$K = -E_{TOT} \quad (A12)$$

$$U_{en} = \frac{7}{3} E_{TOT} - (Z - Q)\mu \quad (A13)$$

$$U_{ee} = -\frac{1}{3} E_{TOT} + (Z - Q)\mu \quad (A14)$$

and so a table of Q , E_{TOT} and $I = -\mu$ together give all the atomic energies. The ionization potential $I = -\mu = dE_{TOT}/dQ$. This data is given in Table 1.

For the neutral free atom, $Q = \mu = 0$ and a numerical calculation yields

$$E_{TOT} = -0.768745 Z^{7/3} \frac{e^2}{a_0} = -20.92 \text{ eV } Z^{7/3} \quad (A15)$$

The limit of highly charged ions is treated analytically by recognizing that when $N_B = Z - Q$ is $\ll Z$, then the nuclear potential dominates and

$$n(r) \approx \frac{1}{3\pi^2} \left(\frac{2Z}{a_0}\right)^{3/2} \left(\frac{R_i - r}{r R_i}\right)^{3/2} \quad (A16)$$

According to Eq. (A6) the volume integral of $n(r)$ must be $Z-Q$, which yields

$$R_i = \frac{a_0}{Z^{1/3}} (18)^{1/3} \left(1 - \frac{Q}{Z}\right)^{2/3} \quad (A17)$$

and hence

$$I = (18)^{-1/3} \frac{e^2}{a_0} \frac{Z^{4/3}}{(1 - Q/Z)^{2/3}} = 10.38 \text{ eV} \frac{Z^{4/3}}{(1 - Q/Z)^{2/3}} \quad (A18)$$

$$E_{TOT} = \frac{3}{(18)^{1/3}} \frac{e^2}{a_0} Z^{7/3} (1 - Q/Z)^{1/3} \quad (A19)$$

These limiting forms illustrate the scaling property discussed in the main text.

The Bloch constant or mean ionization-excitation potential, denoted $\bar{I}$, is conventionally defined as:

$$\log \bar{I} = \frac{1}{Z-Q} \int n(r) \log [\hbar \omega_p(r)] d^3r \quad (A20)$$

where

$$\omega_p(r) = \sqrt{4\pi e^2 n(r)/m} \quad (A21)$$

is the local electron-gas plasma frequency. Equation (A20) for $\bar{I}$ follows from the high-velocity limit of the inhomogeneous electron-gas stopping power according to a formula proposed by Lindhard and Winther. Comparison of calculated values of $\bar{I}$ with experiments shows a substantial discrepancy which may tentatively be attributed to the (unknown) gradient corrections. The Thomas-Fermi values of $\bar{I}$ are too small by a factor of $\sim \sqrt{2}$. A limiting form of $\bar{I}(Z, Q)$ for highly stripped ions is found with the use of Eq. (A16):

$$\bar{I} = (e^{1/2} \sqrt{\frac{8}{9\pi}}) \frac{e^2}{a_0} \frac{Z}{(1 - \frac{Q}{Z})^{1/2}} = 23.86 \text{ eV} \frac{Z}{\sqrt{1 - Q/Z}} \quad (\text{A22})$$

(The symbol e within parentheses is 2.718...).

The dipole polarizability of the Thomas-Fermi ion is calculated by assuming a small perturbation of $n(r)$, $V(r)$ having the form

$$eV_1(r) = \frac{1}{r} f(r) \cos \theta \quad (\text{A23})$$

From Eqs. (A1, A2) we deduce

$$\frac{d^2 f}{dr^2} = \left[\frac{2}{r^2} + K_0^2(r) \right] f(r) \quad (\text{A24})$$

where $K_0(r)$ is determined by the unperturbed density $n_0(r)$:

$$K_0^2(r) = \frac{4}{\pi a_0^3} (3\pi^2 n_0(r))^{1/3} \quad (\text{A25})$$

For $r \rightarrow 0$, the solution is required to be regular. For $r > R_i$, the solution has the form

$$f(r) = Ar^2 + \frac{B}{r} \quad (\text{A26})$$

The first term is the potential of a uniform (homogeneous) applied field $E(\infty)$ and the second is the potential of the induced dipole $P = \alpha E(\infty)$ with

$$\alpha = -\frac{B}{A} \quad (\text{A27})$$

Numerical data for α are given in Table 1. The analytic result for highly charged ions is

$$\alpha = \frac{63}{16} \frac{a_0^3}{Z} \left(1 - \frac{Q}{Z}\right)^3 \quad Q \rightarrow Z \quad (\text{A28})$$

An interesting theorem concerns the penetration of the applied field $E(\infty)$ to the region near the nucleus. The local dipolar field near the nucleus $E(0)$ is determined by examining the

coefficient of r^2 in the series expansion of $f(r)$ near $r = 0$.
The result is

$$\beta = \frac{E(0)}{E(\infty)} = \frac{Q}{2} \quad (\text{A29})$$

Extensive discussions of Thomas-Fermi theory are given by March and Gombas.¹⁶ In recent years, several investigators have examined quantum corrections to the Thomas-Fermi theory which improve the accuracy at the expense of the TF scaling property. Accounts of this work are given by Kalitkin,⁶¹ Kirzhnits,⁶² More² and Schwinger.⁶³

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