

Chapter 1

Charge Equilibrium

Abstract The mean equilibrium charge of a penetrating ion can be estimated on the basis of Bohr's velocity criterion or Lamb's energy criterion. Qualitative and quantitative results are derived on the basis of the Thomas-Fermi model of the atom, which is discussed explicitly. This includes a brief introduction to the Thomas-Fermi-Dirac model. Special attention is paid to trial function approaches by Lenz and Jensen as well as Brandt and Kitagawa. The chapter also offers a preliminary discussion of the role of the stopping medium, gas-solid differences, and a survey of data compilations.

1.1 Introductory Comments

Volume 1 was dedicated to the stopping and scattering of point charges. This provided an opportunity to illustrate fundamental theoretical concepts and procedures. In practice the theory applies to light particles such as electrons and positrons, protons and antiprotons, and heavier ions above a limiting energy which increases rapidly with increasing atomic number.

The restriction to penetrating point charges has been dropped in the present volume. Already about a century ago, Flamm and Schumann (1916) suggested that an alpha particle may capture an electron from the penetrated medium. Henderson (1923) and Rutherford (1924) demonstrated experimentally the presence of singly-charged helium ions in an emerging beam. It was clear that electron capture must be possible for all ions including protons. Conversely, neutral atoms may lose electrons by collisions with the atoms of the penetrated medium.

As a result of a sequence of electron capture and loss events one may expect a penetrating ion to approach a state of dynamical equilibrium around a charge state for which the number of capture events equals the number of loss events per unit time or pathlength in the average. Whether such a state is actually achieved does not only depend on the thickness of the penetrated layer but also on the rate of energy loss, since cross sections for electron capture and loss depend on beam energy.

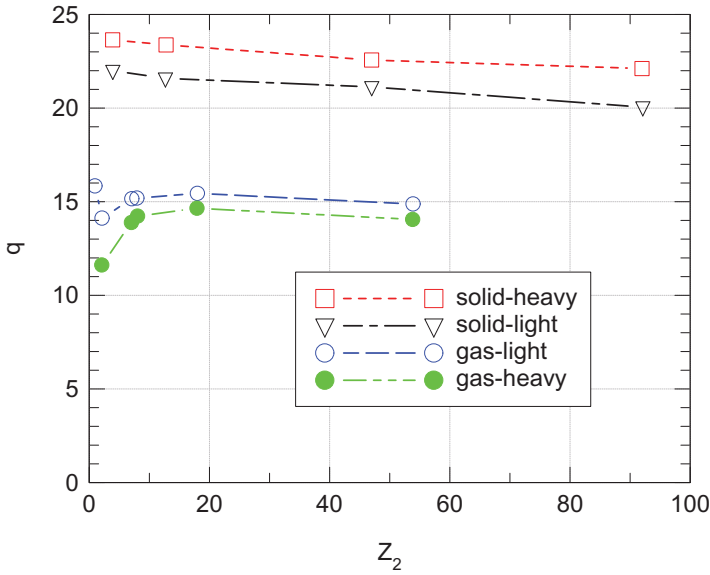


Fig. 1.1 Mean charges of fission fragments penetrating through gaseous targets and emerging from solid targets vs. atomic number Z_2 of the material, according to Lassen (1951b). Separate data are shown for light and heavy fragments

Mean equilibrium charges of alpha particles are close to 2 at energies in the MeV range. Therefore, penetration studies involving composite particles only became urgent with the discovery of nuclear fission (Hahn and Strassmann, 1939, Meitner and Frisch, 1939), where medium-mass heavy ions at MeV energies are involved. Measurements of track lengths of such fission fragments in cloud chambers were performed almost instantaneously by Broström et al. (1940), and a number of now classical papers appeared which addressed the charge and energy loss of those particles (Bohr, 1940, 1941, Lamb, 1940, Knipp and Teller, 1941, Brunings et al., 1941). This early development was summarized by Bohr (1948).

Systematic experimental studies of the charges of fission fragments were initiated by Lassen (1951b,a), who reported a striking difference between solid and gaseous stopping media: Figure 1.1 shows that these ions had mean charges ranging from ~ 11 to 24, which were higher for ions emerging from a solid than for ions penetrating through a gas. This ‘density effect’ became the subject of much lively discussion for almost half a century, starting with early theoretical studies by Bell (1953), Bohr and Lindhard (1954), Neufeld (1954), Gluckstern (1955) and others.

A particularly distressing feature of this density effect, indicated already in Lassen’s early studies but clearly confirmed in later measurements on tandem accelerators by Pierce and Blann (1968), was the near absence of a corresponding density effect in the energy loss. This seeming inconsistency intensified the discussion.

In this monograph the complex of charge-state distributions and charge-dependent stopping has been divided up into three problem areas which will be treated in five

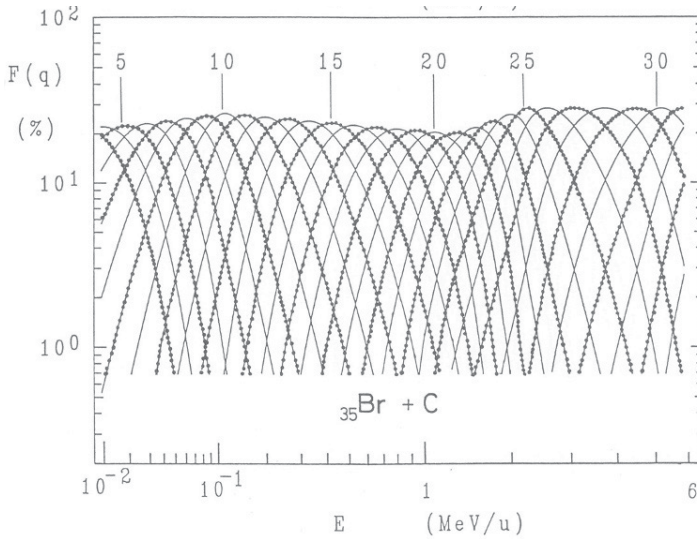


Fig. 1.2 Equilibrium charge fractions for bromine ions in carbon. Numbers above the curves represent the charge number. See text. From Shima et al. (1992)

successive chapters. The present chapter addresses equilibrium charge states without explicit reference to charge-exchange cross sections. Chapter 2 deals with cross sections for electron capture and loss, and Chap. 3 with the associated statistics and energetics. Chapters 4 and 5 deal with the mean energy loss and straggling of swift heavy ions, respectively.

1.2 Qualitative Orientation

Increasing the charge of an ion requires energy. Therefore, as a rough guideline we may assume that the cross section for electron loss decreases with increasing ion charge. Conversely, with decreasing ion charge the capture cross section will decrease and will rapidly approach zero for negative ion charges. Therefore, the probability of a projectile to be in a certain charge state, the *charge fraction*, will have a maximum near some equilibrium charge state and decrease monotonically in both directions.

If the incident charge is higher than the equilibrium charge, capture typically dominates over loss, and vice versa in the opposite case. Remind, however, that charge exchange is a stochastic process: For an individual trajectory, charge fractions can take any value that is compatible with conservation laws.

Figure 1.2 illustrates the situation on the example of Br in C. That figure is based on interpolation and scaling of experimental data by Shima et al. (1992). Numbers above the graphs denote the charge state q . As an example, take $q = 20$, which is

the most abundant one at $E \simeq 1$ MeV/u. Neighbouring charge states 19 and 21 are slightly less abundant, while charge fractions for states 15+ and 25+ are about a factor of 30 lower at that energy.

We may conclude that the distribution in charge-states in equilibrium at a given beam energy may be rather narrow, so that it makes sense to neglect the difference between the average and the peak value and, as a first estimate, to characterize the equilibrium charge state by one number, which in principle depends on the atomic numbers Z_1 and Z_2 of the projectile and the target, respectively, and the beam energy as well as on the physical state of the medium.

1.3 Stripping Criteria

Strictly speaking, the mean equilibrium charge is defined as an average over charge distributions such as those shown in Fig. 1.2. This need not be an integer number. The definition mentioned above requires the average number of capture events per unit time or pathlength to equal the number of loss events. This is already an approximation, since capture and loss cross sections for atoms with a non-integer number of electrons do not make sense. Moreover, databases over cross sections are necessarily incomplete, in particular for condensed stopping media. Therefore, simpler models that do not require quantitative information about cross sections are highly desirable. Let us have a look at options proposed in the literature.

1.3.1 Velocity Criterion

Consider a projectile moving with a velocity v and carrying a number of electrons with orbital speeds v_e . Viewed in a moving reference frame, the projectile is exposed to a beam of target electrons and nuclei. Bohr (1940) divided the projectile electrons into two groups according to whether their orbital speed is greater or smaller than v . Those with orbital speeds significantly smaller than the projectile speed v are relatively weakly bound and will, consequently, have a relatively high ionization cross section and hence be stripped efficiently. Conversely, those with orbital velocities significantly greater than v will tend to respond adiabatically to the disturbance and have only a small chance to be stripped off. The physical content of the adiabaticity criterion has been discussed in Problem 2.19, Vol. 1.

Moreover, you will see in Chap. 2 that electron capture is inefficient when the projectile speed exceeds the orbital speed.

With this we have arrived at the Bohr stripping criterion: In the equilibrium charge state, electrons with orbital velocities $v_e < v$ are stripped off or, in other words: If the projectile carries more electrons initially than predicted by the Bohr stripping criterion, ionization will dominate until the outermost electrons have the orbital speed v .

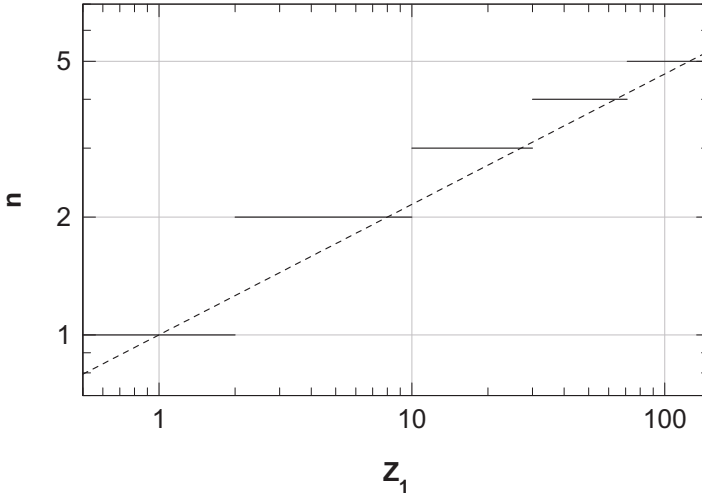


Fig. 1.3 Principal quantum number and shell filling. See text

If the projectile carries fewer electrons than predicted by the Bohr stripping criterion, the outermost electrons will have large orbital velocities. This implies that there are empty states into which electrons can be captured. Hence, capture cross sections will be sizable, while ionization is inefficient.

Equilibrium charge states resulting from the Bohr stripping criterion depend on the adopted atom model. Bohr (1948) argued as follows: Consider an electron in the outermost shell of an ion with the charge $q_1 e$. Within a hydrogenic model, its orbital velocity may be written as

$$v_e \simeq \frac{q_1}{n} v_0, \quad (1.1)$$

where n is the principal quantum number of that shell and $v_0 = c/137$ the Bohr speed.

Figure 1.3 illustrates the filling of shells according to the periodic table. The step-like curve shows the principal quantum number of the outermost occupied shell vs. atomic number Z_1 . Also shown is the curve

$$n = Z_1^{1/3}, \quad (1.2)$$

which approximately connects the upper ends of the steps. With this approximation the Bohr stripping criterion implies

$$v \simeq \frac{q_1}{Z_1^{1/3}} v_0 \quad (1.3)$$

or (Bohr, 1948)

$$q_1 \simeq Z_1^{1/3} \frac{v}{v_0}, \quad (1.4)$$

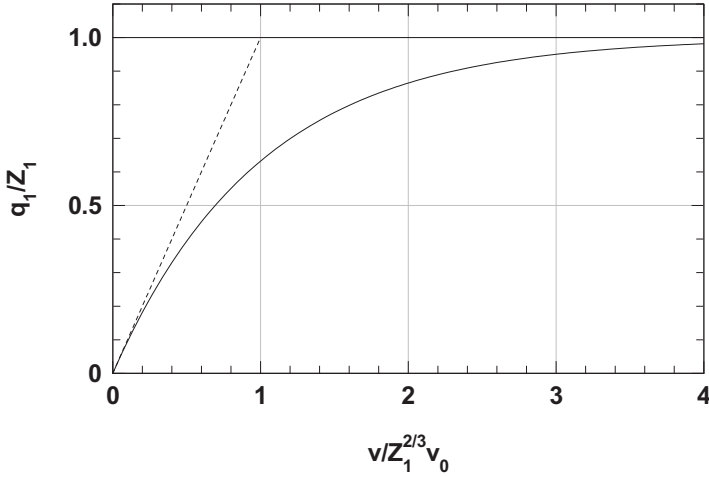


Fig. 1.4 Equilibrium charge fraction vs. projectile speed according to (1.4) and (1.6)

where q_1 denotes the equilibrium charge. However, q_1 cannot increase indefinitely. A plausible way to extend the range of validity of this estimate is to write (1.4) in the form

$$\frac{q_1}{Z_1} \simeq \frac{v}{Z_1^{2/3} v_0}. \quad (1.5)$$

Since q_1/Z_1 cannot exceed unity, we may try a simple extrapolation of (1.4) to arrive at

$$q_1 \simeq Z_1 \left(1 - e^{-v/Z_1^{2/3} v_0} \right), \quad (1.6)$$

as proposed by Pierce and Blann (1968) and shown in Fig. 1.4. You may already have noticed the Thomas-Fermi speed

$$v_{\text{TF}} = Z_1^{2/3} v_0, \quad (1.7)$$

which was mentioned in Sect. 7.2.1, Vol. 1.

While the derivation of these expressions is clearly qualitative, (1.4) and (1.6) compare favourably in general with measured equilibrium charges for a wide variety of projectile-target combinations. Numerous modifications based on empirical data have been made (Betz, 1972), but the Bohr stripping criterion as formulated above is still a useful tool in the field of heavy-ion penetration.

Figure 1.5 shows a more quantitative evaluation of the Bohr criterion. Here, the quantity $\langle v_e^2 \rangle$ has been evaluated for individual shells via tabulated Hartree-Fock wave functions from Clementi and Roetti (1974). For Fluorine and Chlorine you may see 3 and 5 steps, respectively, reflecting subshells of the neutral atom. In bromine and iodine, s and p electrons have been combined for each shell.

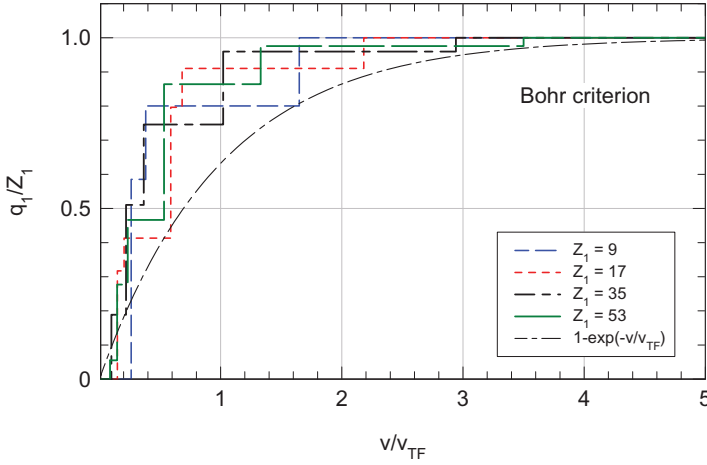


Fig. 1.5 Equilibrium charge fraction vs. projectile speed for halogen ions evaluated from the requirement that $\langle v_e^2 \rangle > v^2$. From Schinner and Sigmund (2014)

1.3.2 Energy Criterion

A different criterion was first introduced by Lamb (1940) who, like Bohr, assumed that loosely-bound electrons are stripped off rapidly. This process is assumed to continue until the most loosely bound electron has a binding energy exceeding $mv^2/2$, the kinetic energy of a free target electron in a reference frame moving with the ion. For a hydrogenic atom, the binding energy of the outermost electron is $= mv_e^2/2$. In that case Lamb's stripping criterion is equivalent with Bohr's.

This criterion may be formulated more quantitatively. Consider a given ion with N_1 electrons. Let its ground-state energy be $E(N_1)$. If the ion moves with a speed v , its total energy will be given as

$$\mathcal{E}(N_1) = E(N_1) + \frac{1}{2}(M_1 + N_1m)v^2, \quad (1.8)$$

where $M_1v^2/2$, the kinetic energy of the nucleus, is taken as a constant in the present context.

Now let N_1 vary: If N_1 is small, the ion will be highly charged and hence have a high energy $E(N_1)$, while $N_1mv^2/2$ is small. If N_1 is large, the ion is nearly neutral, so $E(N_1)$ is low but $N_1mv^2/2$ is large. Hence, $\mathcal{E}(N_1)$ must be expected to have a minimum at N_{eq} , so that

$$\mathcal{E}(N_{eq} \pm 1) > \mathcal{E}(N_{eq}). \quad (1.9)$$

Insertion of (1.8) into (1.9) leads to

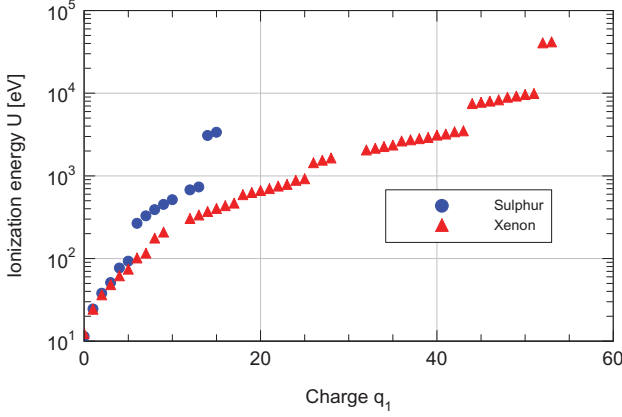


Fig. 1.6 Computed binding energies for all charge states of sulphur and xenon ions according to Carlson et al. (1970). From Schinner and Sigmund (2014)

$$E(N_{\text{eq}}) - E(N_{\text{eq}} + 1) < \frac{1}{2}mv^2 < E(N_{\text{eq}} - 1) - E(N_{\text{eq}}). \quad (1.10)$$

This means that v vs. N_{eq} , and hence q_1 vs. v , has a step-like structure in this model.

The energy criterion assumes that if the ion moves in a medium, collisions with the nuclei and electrons of the target allow the charge of the ion to equilibrate, i.e., to let the ion attain the lowest energy state by losing or capturing electrons. According to (1.8) this state is independent of the properties of the medium, although the time it takes to approach equilibrium must depend on the type of interactions taking place.

For ions with many electrons we may approximate (1.9) by

$$\frac{d\mathcal{E}(N_1)}{dN_1} = \frac{dE(N_1)}{dN_1} + \frac{1}{2}mv^2 = 0 \quad (1.11)$$

for $N_1 = N_{\text{eq}}$. As it stands, both (1.9) and (1.11) involve the assumption that $E(N_{\text{eq}})$ represents the ground state energy of the ion, whatever it is isolated or embedded into a medium. This may be a limitation on the validity of the model, as will be discussed in Sect. 1.5.

Setting $dE(N_1)/dN_1 \simeq U(N_1)$, where $U(N_1)$ is an effective ionization energy of an ion with N_1 electrons, the energy criterion (1.11) reduces to

$$U(N_1) \simeq mv^2/2. \quad (1.12)$$

This is the criterion proposed by Lamb (1940).

Figure 1.6 shows binding energies for all charge states of sulphur and bromine computed by Carlson et al. (1970).

Figure 1.7 shows equilibrium charge states of halogen ions calculated from data like those shown in Fig. 1.7 and (1.12). Steps of the type shown in Fig. 1.3 are still present, although less pronounced.

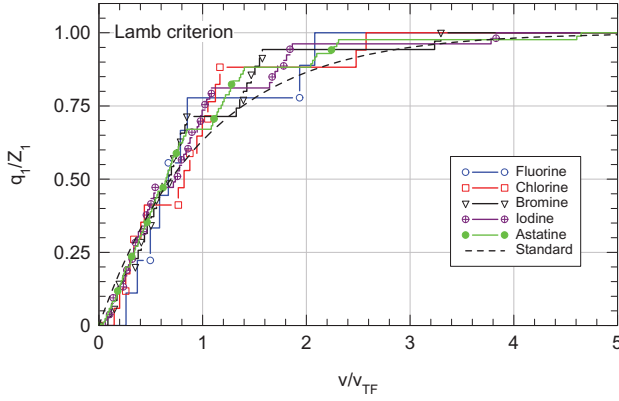


Fig. 1.7 Mean equilibrium charge fractions for halogen ions according to (1.12). The simple formula (1.6) has been included for reference. From Schinner and Sigmund (2014)

1.4 Thomas-Fermi Theory

The energy criterion allows a quantitative evaluation on the basis of the Thomas-Fermi model of the atom, which was briefly introduced in Sects. 7.2.1–7.2.3, Vol. 1, mainly in order to establish scaling relations for stopping parameters. Use will be made more frequently of the model in the present volume dealing with heavier ions, since the accuracy of Thomas-Fermi theory increases with atomic number. Some essential features of the theory will be outlined here, following by and large the presentation of Gombas (1949, 1956).

1.4.1 Thomas-Fermi Equation for an Atomic Ion

The Thomas-Fermi model treats an atom, molecule or even an extended medium as an ensemble of Fermi gases of infinitesimal size of varying density, often called a ‘local density approximation’. The energy of an ion with atomic number Z_1 and N_1 electrons $E(N_1)$ can be expressed as

$$E(N_1) = E^{\text{kin}}(N_1) + E^{\text{Coul}}(N_1) + E^{\text{excor}}(N_1) \quad (1.13)$$

where

$$E^{\text{kin}}(N_1) = \int d^3\mathbf{r} \rho(\mathbf{r}) \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \quad (1.14)$$

is the kinetic energy in accordance with (7.3), Vol. 1 and k_F the Fermi wave number. Making use of the relation $\rho = k_F^3/3\pi^2$, see (5.146), Vol. 1, we may write this in the form

$$E^{\text{kin}}(N_1) = \kappa_k \int d^3\mathbf{r} \rho(\mathbf{r})^{5/3}, \quad (1.15)$$

where

$$\kappa_k = \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} = 2.871 e^2 a_0. \quad (1.16)$$

The electrostatic energy reads

$$E^{\text{Coul}}(N_1) = -Z_1 e^2 \int d^3\mathbf{r} \frac{\rho(\mathbf{r})}{r} + \frac{e^2}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (1.17)$$

One distinguishes between the straight Thomas-Fermi model (Thomas, 1926, Fermi, 1927, 1928) where the exchange-correlation term $E^{\text{excor}}(N_1)$ in (1.13) is ignored, and the Thomas-Fermi-Dirac model (Dirac, 1930) where $E^{\text{excor}}(N_1)$ is determined on the basis of the exchange energy of the Fermi gas.

Explicit calculations will be shown mainly for the straight Thomas-Fermi model ignoring both exchange and correlation. Additional features introduced by exchange will be mentioned briefly. Correlation terms, stemming from higher-order perturbation theory in terms of the Coulomb interaction between electrons affect quantitative details (Gombas, 1943) but will not be considered here. For an estimate of the correlation term being based on many-body electron theory you might consult Hedin and Lundqvist (1969).

In the straight Thomas-Fermi model we have

$$\begin{aligned} \mathcal{E}(N_1) = \kappa_k \int d^3\mathbf{r} \rho(\mathbf{r})^{5/3} - Z_1 e^2 \int d^3\mathbf{r} \frac{\rho(\mathbf{r})}{r} \\ + \frac{e^2}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{2}(M_1 + N_1 m)v^2. \end{aligned} \quad (1.18)$$

We wish to find an electron density $\rho(\mathbf{r})$ which minimizes $\mathcal{E}(N_1)$. Once that function has been determined we may find the number of electrons by integration,

$$N_1 = \int d^3\mathbf{r} \rho(\mathbf{r}). \quad (1.19)$$

This differs from the standard presentations of Thomas-Fermi theory (Gombas, 1949, 1956), where the ion charge is given, so that (1.19) represents a boundary condition which enters into the scheme via a Lagrange parameter.

For an infinitesimal variation $\delta\rho(\mathbf{r})$ we find the change in energy $\delta\mathcal{E}(N_1)$,

$$\begin{aligned} \delta\mathcal{E}(N_1) = \int d^3\mathbf{r} \delta\rho(\mathbf{r}) \\ \left(\frac{5}{3}\kappa_k \rho(\mathbf{r})^{2/3} - \frac{Z_1 e^2}{r} + e^2 \int d^3\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{2}mv^2 \right), \end{aligned} \quad (1.20)$$

and hence, from $\delta\mathcal{E}(N_1) = 0$,

$$\frac{5}{3}\kappa_k\rho(\mathbf{r})^{2/3} - \frac{Z_1e^2}{r} + e^2 \int d^3\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{2}mv^2 = 0. \quad (1.21)$$

Now, the quantity

$$\phi(r) = \frac{Z_1e}{r} - e \int d^3\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (1.22)$$

represents the potential seen by a test charge. With this, (1.21) may be written in the form

$$\rho(r) = \left(\frac{3}{5\kappa_k} \right)^{3/2} \left[e\phi(r) - \frac{1}{2}mv^2 \right]^{3/2}. \quad (1.23)$$

Expressing $\rho(r)$ by Poisson's equation $\nabla^2\phi(r) = 4\pi e\rho(r)$ you finally arrive at

$$\nabla^2[\phi(r) - \phi_0] = 4\pi e\sigma_0[\phi(r) - \phi_0]^{3/2}, \quad (1.24)$$

where

$$\phi_0 = \frac{mv^2}{2e} \quad (1.25)$$

and

$$\sigma_0 = \left(\frac{3e}{5\kappa_k} \right)^{3/2} = 0.09553 \left(\frac{me}{\hbar} \right)^{3/2}. \quad (1.26)$$

Equation (1.24) is the well-known Thomas-Fermi equation introduced in Sect. 7.2.3, Vol. 1. This includes the quantity ϕ_0 which, in the standard case of N_1 being predetermined, represents a Lagrange parameter. In the present context, ϕ_0 is predetermined via the projectile speed according to (1.25).

1.4.2 Solution

Following Gombas (1949) again you may write the potential in the form

$$\phi(r) - \phi_0 = \frac{Z_1e}{r} g(\xi), \quad (1.27)$$

where $\xi = r/a$. Here a is a screening radius which may be chosen such as to incorporate all dependence on atomic number. If so, $g(\xi)$ will be a universal screening function.

Noting that

$$\nabla^2 = \frac{1}{r} \frac{d^2}{dr^2} r \quad (1.28)$$

for a spherically symmetric function, you may rewrite (1.24) in the form (cf. Problem 1.1)

$$\frac{d^2 g(\xi)}{d\xi^2} = \frac{C_1}{\xi^{1/2}} g(\xi)^{3/2} \quad (1.29)$$

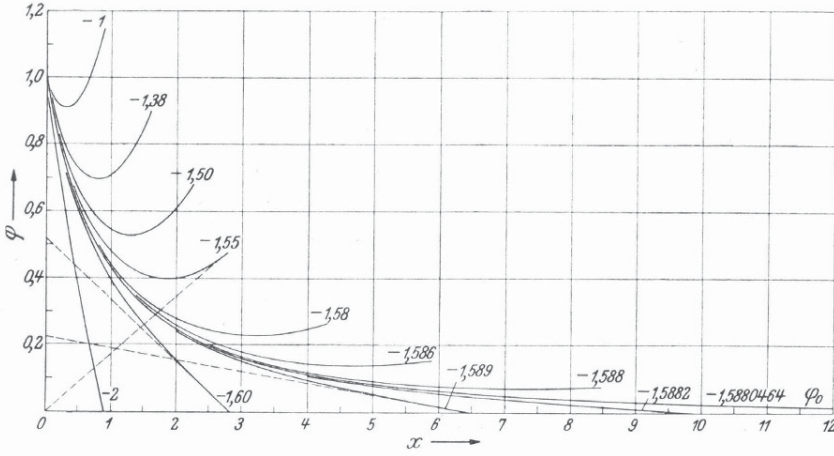


Fig. 1.8 Solutions of the Thomas-Fermi equation (1.31) for $g(0) = 1$. Numbers at the curves indicate the values of $dg(\xi)/d\xi|_{\xi=0}$. From Gombas (1949)

with

$$C_1 = \left[2 \left(\frac{4}{3\pi} \right)^{2/3} \frac{a Z_1^{1/3}}{a_0} \right]^{3/2}, \quad (1.30)$$

where $a_0 = \hbar^2/m e^2$ is the Bohr radius and use has been made of (1.16) and (1.26).

We may define the screening radius a such that $C_1 = 1$. With this the Thomas-Fermi equation reduces to

$$\frac{d^2 g(\xi)}{d\xi^2} = \frac{g(\xi)^{3/2}}{\xi^{1/2}} \quad (1.31)$$

and

$$a = a_{\text{TF}} = 0.8853 a_0 Z_1^{-1/3}, \quad (1.32)$$

which defines the numerical constant quoted in (7.15), Vol. 1.

Equation (1.31) can be solved if two constants are given. Since $\phi(r)$ must approach the Coulomb potential close to the nucleus we have

$$g(0) = 1. \quad (1.33)$$

Figure 1.8 shows solutions for various values of $g'(0) = dg(\xi)/d\xi|_{\xi=0}$. You may notice that the shape of the solutions is quite sensitive to the value of $g'(0)$. As $-g'(0)$ increases, the integral under the curves decreases. Remembering (1.19), you may expect this quantity to be uniquely related to the number of electrons surrounding the nucleus.

Inspection of (1.23) indicates that there is a point r_0 for which

$$e\phi(r_0) = \frac{1}{2}mv^2 \quad (1.34)$$

and hence $\rho(r_0) = 0$, so that $\rho(r) = 0$ for $r > r_0$, assuming that $\phi(r)$ falls off monotonically. Outside r_0 we must have a Coulomb potential with the ion charge q_1 ,

$$\phi(r) = \frac{(Z_1 - N_1)e}{r} \quad \text{for } r \geq r_0 \quad (1.35)$$

and, at $r = r_0$,

$$\phi(r_0) = \frac{(Z_1 - N_1)e}{r_0} = \phi_0, \quad (1.36)$$

where the last identity follows from (1.27). Thus, the charge number q_1 is given by

$$q_1 = Z_1 - N_1 = \frac{r_0\phi_0}{e} = \frac{r_0mv^2}{2e^2} \quad (1.37)$$

In Thomas-Fermi units this reads

$$\frac{q_1}{Z_1} = \frac{0.8853}{2} \xi_0 \frac{v^2}{v_{\text{TF}}^2}, \quad (1.38)$$

where $v_{\text{TF}} = v_0 Z_1^{2/3}$ is the Thomas-Fermi speed.

Equation (1.38) provides the connection between the ion charge and the beam velocity, once the Thomas-Fermi equation has been solved for a given value of $g'(0)$. The connection between $g'(\xi_0)$ and q_1 or N_1 is found from

$$N_1 = \int_{0 < r \leq r_0} d^3r \rho(r) = \frac{1}{4\pi e} \int_{0 < r \leq r_0} d^3r \nabla^2 \phi(r). \quad (1.39)$$

After inserting (1.27) and $r = a\xi$ this reads

$$N_1 = Z_1 \int_{0+}^{\xi_0} d\xi \xi g''(\xi) = Z_1 \left(\xi g'(\xi) - g(\xi) \right)_0^{\xi_0}, \quad (1.40)$$

where $\xi_0 = r_0/a$. With $g(0) = 1$ and $g(\xi_0) = 0$ this reduces to

$$\xi_0 g'(\xi_0) = -\frac{q_1}{Z_1}. \quad (1.41)$$

Equations (1.36) and (1.41) also follow from the standard treatment, where N_1 is predetermined and the atom at rest (Gombas, 1949, 1956). This implies that the relation between the charge distribution $\rho(r)$ and the number of electrons N_1 is independent of the projectile speed. In other words, in the present description, the ion charge depends on the projectile speed, while the electron density reflects the ground-state configuration of the ion for the given ion charge, whatever the projectile speed.

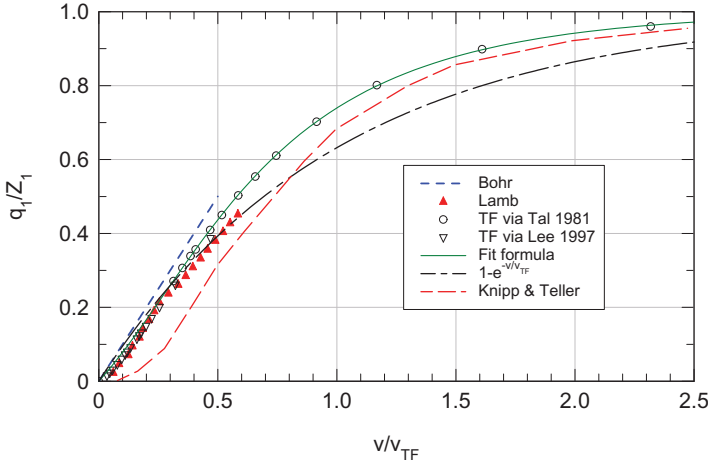


Fig. 1.9 Equilibrium charge fraction q_1/Z_1 of a free Thomas-Fermi ion vs. velocity. Dots: Evaluated from numerical tabulations (Tal and Levy, 1981, Lee and Wu, 1997) of Thomas-Fermi functions for different charge states; also included is Bohr's estimate (1.5), the results given by Lamb (1940) and by Knipp and Teller (1941) as well as (1.42) and (1.6)

Accurate tabulations of the Thomas-Fermi function for varying charge numbers are available. Dots in Fig. 1.9 were found from tables by Tal and Levy (1981) and by Lee and Wu (1997). This result is equivalent with that of Yarlagadda et al. (1978). It is seen to be well represented by a fitting formula

$$\frac{q_1}{Z_1} = \frac{1 - e^{-1.43v/Z_1^{2/3}v_0}}{1 + e^{-3.56v/Z_1^{2/3}v_0}}. \quad (1.42)$$

Small deviations from the result of Lamb (1940) are presumably due to inaccuracies of the Thomas-Fermi functions available at the time. The behaviour at low speed ($v \ll v_{TF}$) is represented by Bohr's expression, $q_1 = Z_1^{1/3}v/v_0$, multiplied by 0.725. Deviations from the frequently-used exponential curve (1.6) are, however, noticeable. The result of Knipp and Teller (1941), based on the velocity criterion, differs significantly, in particular at low speed.

1.4.3 Trial Function Approach

Variational principles are frequently explored by means of trial functions. In Thomas-Fermi theory, the first ansatz goes back to Lenz (1932) and Jensen (1932). Before reporting specific results, let us first look at a rather general formulation, setting

$$\rho(\mathbf{r}) = \frac{N_1}{a^3} f(\xi), \quad (1.43)$$

where $\xi = r/a$ and

$$\int 4\pi\xi^2 d\xi f(\xi) = 1. \quad (1.44)$$

The Thomas-Fermi-Dirac energy, (1.18), reads

$$\mathcal{E} = A_1 \frac{N_1^{5/3}}{a^2} - A_2 \frac{Z_1 N_1}{a} + A_3 \frac{N_1^2}{a} - A_4 \frac{N_1^{4/3}}{a} + N_1 \frac{mv^2}{2}, \quad (1.45)$$

where

$$A_1 = \kappa_k \int_0^\infty 4\pi\xi^2 d\xi f(\xi)^{5/3}, \quad (1.46)$$

$$A_2 = e^2 \int_0^\infty 4\pi\xi d\xi f(\xi), \quad (1.47)$$

$$A_3 = e^2 \int_0^\infty 4\pi\xi d\xi f(\xi) \int_0^\xi 4\pi\xi'^2 d\xi' f(\xi'), \quad (1.48)$$

$$A_4 = \kappa_a \int_0^\infty 4\pi\xi^2 d\xi f(\xi)^{4/3}. \quad (1.49)$$

In the Ritz procedure, the function $f(\xi)$ is not varied freely but will be given some form which is expected to be more or less realistic. It may contain variational parameters. N_1 and a are independent variational parameters.

If $f(\xi)$ does not contain additional parameters, minimization of (1.45) with respect to N_1 and a yields

$$\frac{\partial \mathcal{E}}{\partial N_1} = \frac{5A_1}{3} \frac{N_1^{2/3}}{a^2} - A_2 \frac{Z_1}{a} + 2A_3 \frac{N_1}{a} - \frac{4A_4}{3} \frac{N_1^{1/3}}{a} + \frac{mv^2}{2} = 0 \quad (1.50)$$

$$\frac{\partial \mathcal{E}}{\partial a} = -2A_1 \frac{N_1^{5/3}}{a^3} + A_2 \frac{Z_1 N_1}{a^2} - A_3 \frac{N_1^2}{a^2} + A_4 \frac{N_1^{4/3}}{a^2} = 0. \quad (1.51)$$

Here, (1.51) provides a connection between the screening radius and the number of electrons which is independent of v , as was found in the previous section in case of the exact solution. Equation (1.50) specifies the connection between N_1 and the speed v .

Let us have a look at limiting cases. For a bare ion, $N_1 = 0$, you readily verify from (1.51) that $a = 0$ and, consequently, $v = \infty$ according to (1.50). For a neutral ion, $N_1 = Z_1$, you may expect $v = 0$, but this is not generally the case. In the Thomas-Fermi case where $A_4 = 0$ you find

$$a = \frac{2A_1}{(A_2 - A_3)Z_1^{1/3}} \quad (1.52)$$

$$\frac{mv^2}{2} = \frac{(A_2 - A_3)(A_2 - 7A_3)Z_1^{4/3}}{12A_1}. \quad (1.53)$$

Table 1.1 Parameters entering Ritz variational procedure. See text

	$f(\xi)$	$mA_1/\hbar^2$	A_2/e^2	A_3/e^2	A_4/e^2	$(A_2 - 7A_3)/e^2$
Lenz-Jensen	$\exp(-\xi^{1/2})/16\pi\xi^{3/2}$	0.06324	0.5	0.0625	0.05629	0.0625
Yukawa	$\exp(-\xi)/4\pi\xi$	0.24000	1.0	0.2500	0.17756	-0.7500
Exponential	$\exp(-\xi)/8\pi$	0.03614	0.5	0.2969	0.10638	-1.5781

If we assume that a neutral ion is the most stable configuration at low speed we must have

$$A_2 \geq 7A_3, \quad (1.54)$$

and if we want $q_1(v = 0) = Z_1$ we must have

$$A_2 = 7A_3. \quad (1.55)$$

Inspection of (1.47) and (1.48) shows that this condition only involves the function $f(\xi)$, independent of N_1 and a .

Equation (1.55) is a fairly strong requirement. In the Thomas-Fermi-Dirac model, where A_4 is taken into account you find, for $N_1 = Z_1$,

$$a = \frac{2A_1}{(A_2 - A_3 + A_4 Z_1^{-2/3})Z_1^{1/3}}, \quad (1.56)$$

$$\frac{mv^2}{2} = \frac{(A_2 - A_3 + A_4 Z_1^{-2/3})(A_2 - 7A_3 + 3A_4 Z_1^{-2/3})Z_1^{4/3}}{12A_1}, \quad (1.57)$$

i.e.,

$$A_2 = 7A_3 - 3A_4/Z_1^{2/3}. \quad (1.58)$$

This may give a hint on how to incorporate an explicit Z_1 dependence into a trial function for the Thomas-Fermi-Dirac case.

1.4.4 Examples of Trial Functions

A successful variational procedure involving trial functions was developed by Lenz (1932) and Jensen (1932). In the present notation their charge density may be expressed through (1.43) with

$$f(\xi) = \text{const} \frac{\exp(-\xi^{1/2})}{\xi^{3/2}} \left(\sum_{j=0}^n c_j \xi^{j/2} \right), \quad (1.59)$$

where $c_0 = 1$ and c_j for $j = 1 \dots n$ are additional variational parameters. In practice n was set to either zero or 1.

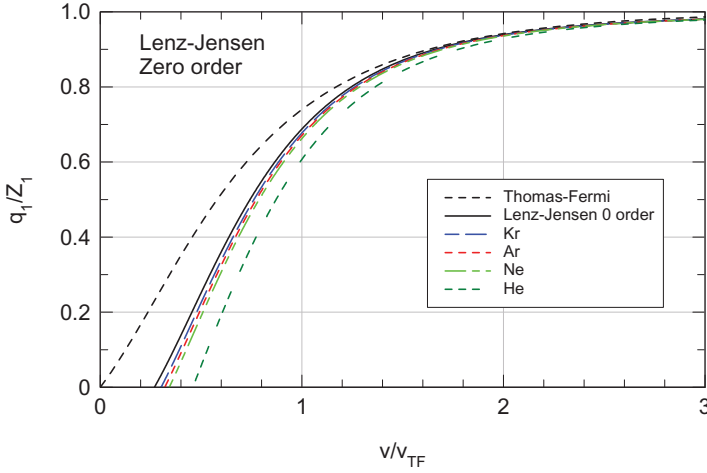


Fig. 1.10 Mean equilibrium charge fraction q_1/Z_1 in statistical theory. The dot-dashed line is the Thomas-Fermi curve shown in Fig. 1.9. The solid line results from the zero-order Lenz-Jensen model ($c_j = 0$ for $j \geq 1$). The four lines in colour are based on the same model but include the exchange term in accordance with the Thomas-Fermi-Dirac model. The dashed curve ('LJ corrected') neglects exchange but was constructed by multiplying A_3 by a factor $8/7$

Results for the case of $n = 0$ are compared in Table 1.1 together with two other examples,

- a Yukawa function (Brandt and Kitagawa, 1982),

$$\rho(r) = \frac{N_1}{4\pi a^2 r} e^{-r/a}, \quad (1.60)$$

and

- a simple exponential

$$\rho(r) = \frac{N_1}{8\pi a^3} e^{-r/a}. \quad (1.61)$$

In addition to the coefficients A_j , $j = 1, \dots, 4$, also the expression $A_2 - 7A_3$ has been included in Table 1.1. This quantity is positive but small for Lenz-Jensen interaction, indicating that N_1 does not drop completely to zero as v approaches zero. This reflects the fact that for an atom or ion at rest, the c_1 term cannot be neglected (Gombas, 1949).

Conversely, for the two other trial functions, $A_2 - 7A_3$ is negative and substantial. Although adding the A_4 -term provides a correction in the desired direction, it is far from large enough to generate a physically acceptable picture. This discourages any attempt to determine equilibrium charges with one of these trial functions on the basis of the Lamb criterion.

Figure 1.10 shows results for the Lenz-Jensen model. All curves are found to lie below the Thomas-Fermi result shown in Fig. 1.9. The straight zero-order Lenz-Jensen result shows q_1 to drop below zero at $v \simeq v_{TF}/3$. The dashed curve ('LJ

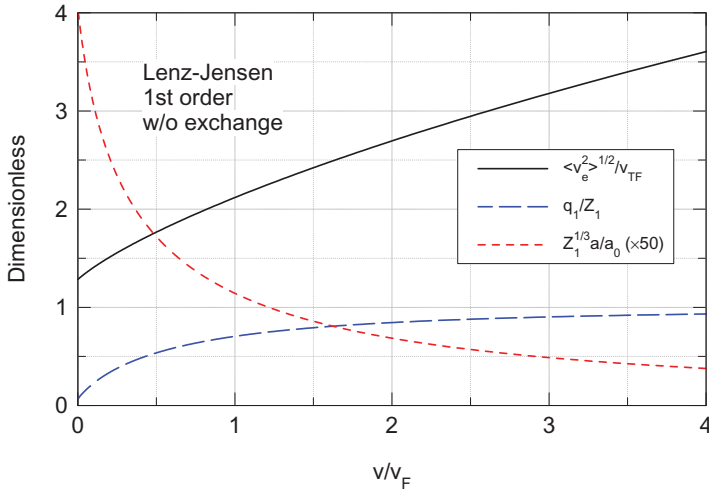


Fig. 1.11 First-order Lenz-Jensen approximation. Solid curve: Rms orbital velocity vs. beam speed according to Schinner and Sigmund (2014). Dashed curve: Charge fraction. Dotted curve: Screening radius. All in Thomas-Fermi units

corrected') was found by multiplying A_3 by $8/7$, thus forcing q_1 to approach zero at $v = 0$. This is just to indicate that the behaviour of these curves at low charge states/beam velocities is quite sensitive to minor modifications of the input.

Also included in the graph are four curves including exchange. As noticed already, the exchange correction is quite small except for helium, but it moves the curves away from the origin rather than towards it.

Finally, let us have a look at the first-order Lenz-Jensen approximation. For $c_1 \neq 0$, c_1 is treated as an additional variational parameter, which adds a third equation to (1.50) and (1.51). You find some hints in Problem 1.6.

Figure 1.11, which is based on this approximation, shows a significantly more reasonable behaviour of the charge fraction at low projectile speed, as compared to the zero-order result from Fig. 1.10. Also shown is the rms orbital speed vs. projectile speed according to Schinner and Sigmund (2014). While this is not the speed that is entering the Bohr stripping criterion, the two speeds are evidently not unrelated.

1.4.5 Brandt-Kitagawa Theory

It is evident from Table 1.1 that the Yukawa potential is not a suitable trial function in connection with the straight Thomas-Fermi model. Nevertheless, Brandt and Kitagawa (1982) proposed a description, based on this trial function, which has been utilized with considerable success. How is this possible? Well, the problem

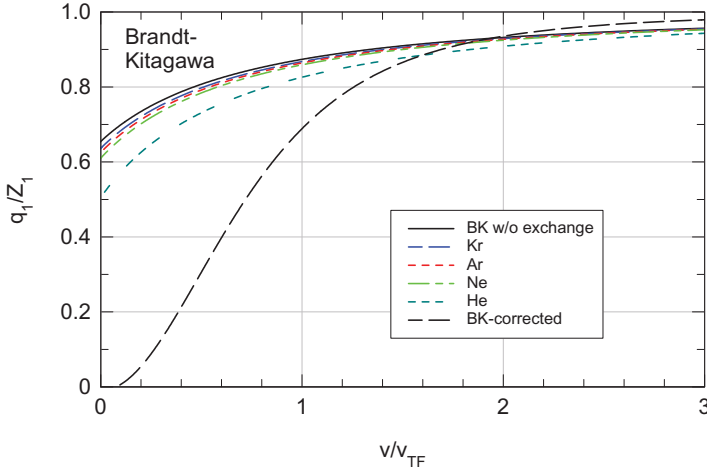


Fig. 1.12 Same as Fig. 1.10 for Yukawa trial function. Solid curve ('BK w/o exchange'): Full Coulomb interaction without exchange and correlation. Dashed curve ('BK corrected'): Coulomb interaction reduced by factor $4/7$. Dashed coloured lines: Including exchange for Kr, Ar, Ne, He (top to bottom)

lies in the quantity $A_2 - 7A_3$ which, according to Table 1.1, is nonvanishing, so the projectile is not neutral for $v = 0$, see Fig. 1.12.

Brandt and Kitagawa (1982) proposed to force the quantity $A_2 - 7A_3$ to vanish by reducing the Coulomb energy of the electron gas by a factor of $4/7$. They argued that the exchange-correlation energy lowers the Coulomb interaction and that, in the average, this could be accounted for by a constant factor. The result is shown as the dashed curve in Fig. 1.12. It was also demonstrated, by comparison with the Lenz-Jensen function, that energy and screening versus charge state showed a reasonable behaviour.

Despite this success, there are obvious objections:

1. If $A_1 - 7A_2$ differs significantly from zero, this indicates a weak point in the trial function, not in the expression for the energy.
2. The exchange-correlation energy of the Fermi gas is here treated as output rather than as input, as it should in a variational calculation where the electron density is the variable.
3. According to Table 1.1 as well as Fig. 1.12 the relative magnitude of the exchange term is much smaller than the necessary correction, and the correlation term is even smaller.

A critical discussion of the model of Brandt and Kitagawa was presented by Mathar and Posselt (1995), where also possible modifications by taking into account the orbital motion of the target electrons were analyzed.

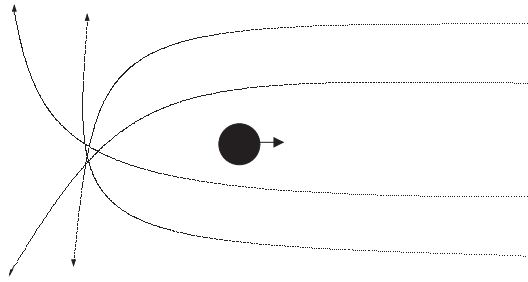


Fig. 1.13 Pile-up of electron trajectories behind a moving ion. See text

1.5 Effect of the Stopping Medium

Up to this point the charge state of a moving ion has been considered as independent of the medium. However, as mentioned in Sect. 1.1, a significant gas-solid difference in the equilibrium charge of fission fragments was observed long ago by Lassen (1951b,a). One may assume that differences of this kind are more general, and that dependencies on other physical and chemical properties of the target might exist.

We shall see in Chap. 3 that cross sections for electron capture and loss play a central role in the theoretical interpretation of the gas-solid effect observed for fission fragments and other swift heavy ions. However, even within the present picture, where we look at the minimum-energy state of a moving ion, the stopping medium has an influence by modifying the Coulomb potential of the projectile and thus the energy levels of bound electrons.

An early hint on such an influence is due to Neufeld and Snyder (1957). Figure 1.13 shows the situation in the rest frame of the projectile. Here the projectile is exposed to a homogeneous current of target electrons which experience its attractive force and hence are deflected toward the ion trajectory. As a consequence there will be collected an excess negative charge behind the ion.

Neufeld and Snyder (1957) asserted that the repulsive potential determined by this negative charge will give rise to expulsion of projectile electrons and, hence, to an increased ion charge state. The magnitude of this effect must increase with increasing density of the stopping material.

1.5.1 Linear Theory

One way of studying this effect is by use of the polarization potential discussed in Chap. 5, Vol. 1,

$$\Phi_{\text{ind}}(\mathbf{r}, t) = \frac{Z_1 e}{2\pi^2} \int \frac{d^3 \mathbf{k}}{k^2} e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{v}t)} \left(\frac{1}{\varepsilon(\mathbf{k}, \omega)} - 1 \right) \quad (1.62)$$

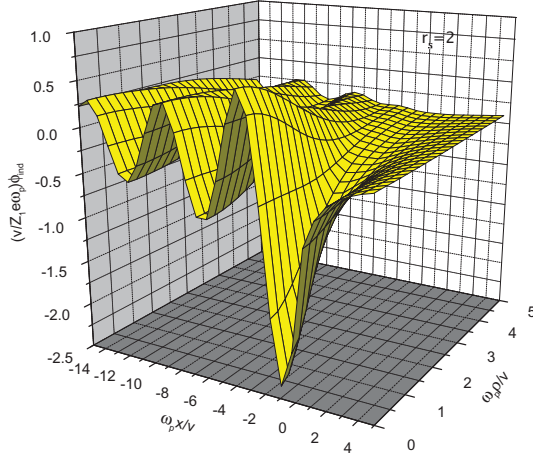


Fig. 1.14 Induced potential for Fermi gas at $B = 2mv^2/\hbar\omega_p = 10$ and $r_s = 2$. From Schinner and Sigmund (2012)

according to Lindhard (1954), where $\varepsilon(k, \omega)$ is the dielectric function which is most often taken to be the one for a Fermi gas of density ρ .

The polarization (or *wake*) potential has been discussed extensively in connection with the penetration of molecules and clusters. Therefore, a detailed discussion will be found in Chap. 10. Only some selected results will be shown here.

The potential (1.62) has cylindrical symmetry. Therefore, introducing cylindrical coordinates (x, ρ) and viewing the situation from a reference frame moving with the projectile velocity $\mathbf{v}$, we may write the induced potential in the form introduced by Neufeld and Ritchie (1955),

$$\Phi_{\text{ind}}(x, \rho) = \frac{Z_1 e}{\pi} \int_0^\infty k \, dk \, J_0(k\rho) \int_{-\infty}^\infty \frac{e^{i\kappa x} \, d\kappa}{k^2 + \kappa^2} \times \left(\frac{1}{\varepsilon(\sqrt{k^2 + \kappa^2}, \kappa v)} - 1 \right), \quad (1.63)$$

where J_0 indicates a Bessel function in standard notation (Abramowitz and Stegun, 1964).

Numerous graphs from the literature show wake potentials calculated from this or related models (Echenique et al., 1990). Figure 1.14 shows a three-dimensional picture of the induced potential of a point charge moving at $B = 2mv^2/\hbar\omega_p = 10$ through a Fermi gas with an electron density ρ characterized by a Wigner-Seitz radius $r_s = 2$, where

$$\frac{4\pi}{3}(r_s a_0)^3 \rho = 1. \quad (1.64)$$

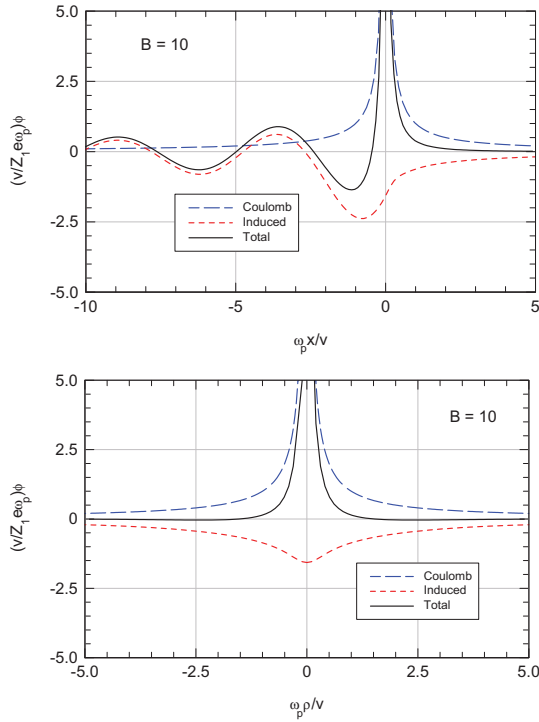


Fig. 1.15 The induced potential shown in Fig. 1.14 in the plane $\rho = 0$ (top) and $x = 0$ (bottom), together with the bare Coulomb potential and the total potential. From Schinner and Sigmund (2012)

The Fermi gas has been described by the dielectric function of Lindhard (1954), (5.154)–(5.156), Vol. 1.

Figure 1.15 shows the induced potential, the Coulomb potential and the sum of the two, the potential seen by a test charge. Two prominent features are evident in the total potential. Near the projectile the Coulomb potential is screened asymmetrically. Further away, at some distance behind the projectile, the potential is dominated by the induced potential.

Consider first the behaviour of the potential in the vicinity of the projectile near $x = \rho = 0$. Here the induced potential tends to screen the Coulomb potential. Figure 1.15 shows that screening is lacking forward-backward symmetry and, moreover, varies from the longitudinal to the transverse plane. Comparison with Fig. 1.16 indicates that the variation with projectile speed is negligible in the transverse and the forward direction — when visualized in the proper scaled variable $\omega_p \rho / v$ — while the variation in the backward direction is noticeable.

We may draw the qualitative conclusion that screening of the Coulomb potential must reduce the number of bound states. Therefore, in the absence of other effects, the induced potential must tend to decrease the number of bound electrons.

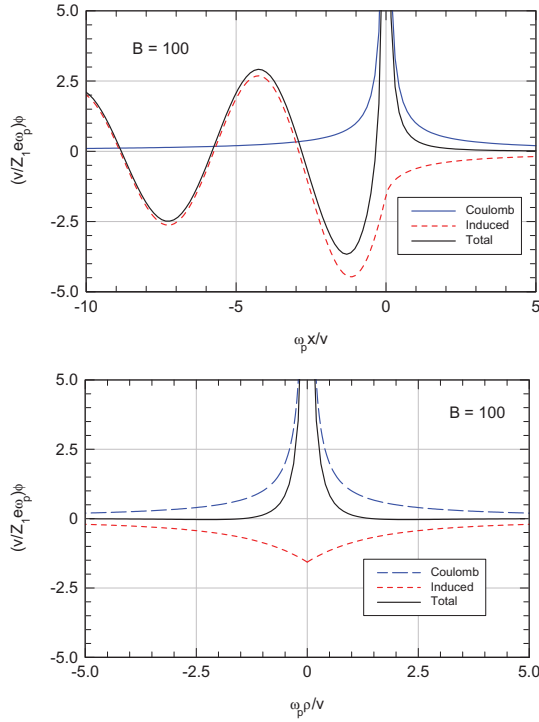


Fig. 1.16 Same as Fig. 1.15 for $B = 2mv^2/\hbar\omega_p = 100$. From Schinner and Sigmund (2012)

1.5.2 Application to Light Ions

Quantitative estimates in the literature have focused on protons, following pioneering work by Neelavathi et al. (1974). Key questions have been:

1. Under which conditions can a proton moving through an electron gas bind an electron, and
2. Under which conditions can a proton bind two electrons.

An illuminating review of this aspect has been provided by Arista (2006). With a focus on projectile speeds well below the Fermi velocity, theoretical tools employed in those studies were taken from condensed-matter physics, going far beyond the simple linear theory sketched in the previous section.

In addition to a careful review of the literature, where there are mutually conflicting results, Arista (2006) presented simple estimates based on a nonlinear theory of the Fermi gas which is to be discussed in Chap 8. This theory involves the Friedel sum rule, which is discussed in Appendix 8.10.2 and operates with three trial functions for the potential of a proton embedded in the electron gas.

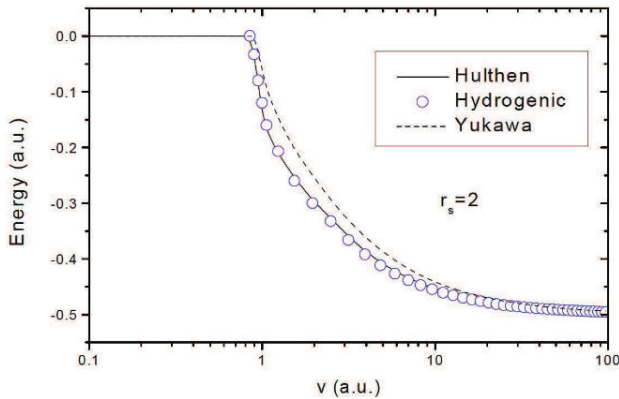


Fig. 1.17 Binding energy of an electron state around a proton moving in a Fermi gas ($r_s = 2$) at a speed v . Atomic units v_0 and e^2/a_0 . From Arista (2006)

The main result of such an estimate — which is supported by experimental evidence — is shown in Fig. 1.17, indicating that a bound state exists only for $v \gtrsim v_0$, and that the binding energy of neutral hydrogen in vacuum is reached at v/v_0 above 10. Results based on the three trial functions for the potential, each of which being characterized by one variational parameter, the screening radius, are in close agreement with each other.

Arista (2006) concludes that ‘slow protons in metals behave as free particles dressed by a screening cloud of conduction electrons’, while bound states appear at higher velocities.

1.5.3 Wake-Riding Electrons

The oscillatory structure behind the ion which you have seen in Figs. 1.14–1.16 has given rise to lively discussions in the literature. One interesting aspect is the question of whether electrons could be trapped in bound states in the first or higher potential maxima (Neelavathi et al., 1974) — i.e., in the minima of the potential energy of electrons — where the potential has a quasi-paraboloidal shape. Such a ‘wake-riding’ electron would be expected to leave the target about simultaneously with the projectile ion, and since it cannot any longer be expected to be bound, it would be recordable as a free electron with the velocity of the emerging ion and with a direction close to that of the ion beam.

However, energy spectra of electrons emitted by swift ions emerging from a solid target show signatures of a wide variety of processes, which will be the subject of a chapter in Volume 3. In the present context, *cusp* or *convoy* electrons are of interest. The term ‘cusp’ refers to the narrow distribution in both energy and direction of

these electrons. The term ‘convoy’ refers to an original prediction (Neelavathi et al., 1974) of wake-riding electrons.

Cusp electrons have been observed in numerous experiments in both solids and gases, and relevant processes include both electron capture and electron loss into the continuum (Macek, 1970). Experimental evidence (Laubert et al., 1978, Meckbach et al., 1977, Breinig et al., 1982, Kroneberger et al., 1996) appears to favour the latter processes rather than wake-riding. However, regardless of the specific interpretation, the very fact that electrons are emitted with a velocity close to that of the projectile indicates proximity in space. While such electrons contribute to the screening of the ionic potential, their number is usually considerably less than one electron per ion.

Calculated electronic binding energies in such states depend on the material and the projectile speed (Neelavathi et al., 1974, Flores and Echenique, 1991). For 2.5 MeV protons, Neelavathi et al. (1974) quote 4.08 eV in aluminium. For $v = 0.8v_0$, Salin et al. (1999) quote 136 eV in an electron gas with $r_s = 2.07$. Considering either Bohr’s or Lamb’s stripping criteria, the lifetime of wake-riding electrons must be quite short.

1.5.4 Effect of Screening

Now, consider the effect of projectile screening on the charge state of a heavier ion. Following Schinner and Sigmund (2014) we ignore forward-backward asymmetry of the screening radius and set the potential to

$$\phi(r) \simeq \frac{Z_1 e}{r} e^{-\omega r/v}, \quad (1.65)$$

as was done by Lindhard (1976) in a different context. Since we are concerned about the potential in the vicinity of the nucleus, we may approximate

$$\phi(r) \simeq \frac{Z_1 e}{r} \left(1 - \frac{\omega r}{v}\right), \quad (1.66)$$

assuming the projectile speed to be high enough so that v/ω is large compared to the effective projectile radius. Here, ω is an effective plasma frequency of the medium.

This implies that a term

$$\int d^3r \rho_e(\mathbf{r}) \left(\frac{-Z_1 e \omega}{v} \right) = -Z_1 N_1 e^2 \frac{\omega}{v} \quad (1.67)$$

has to be added to the energy $\mathcal{E}(N_1)$ in (1.18). This leaves (1.51) unchanged but adds an additional term to (1.50). Since (1.65) represents an expansion up to first order in ω/v , it is appropriate also to solve the resulting cubic equation for N_1/Z_1 ,

$$\frac{v^2}{v_{TF}^2} = \xi^2 - \eta \frac{v_{TF}}{v} \quad (1.68)$$

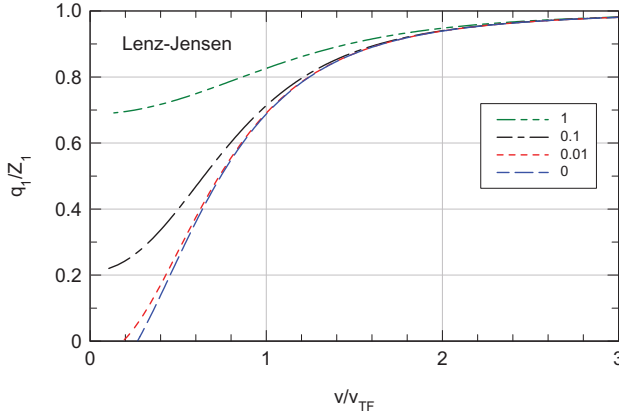


Fig. 1.18 Influence of the stopping medium on the equilibrium charge according to the Lamb criterion applied to a Lenz-Jensen trial function. Evaluated from (1.15). Labels of the curves indicate the value of η , (1.70). From Schinner and Sigmund (2014)

with

$$\xi^2 = \frac{(A_2 - 7A_3N_1/Z_1)(A_2 - A_3N_1/Z_1)}{6A_1(N_1/Z_1)^{2/3}mv_0^2} \quad (1.69)$$

and

$$\eta = \frac{2\hbar\omega}{Z_1mv_0^2} \quad (1.70)$$

by expansion up to the first order in ω/v . Then,

$$\frac{v^2}{v_{TF}^2} \simeq \xi^2 - \frac{\eta}{\xi}. \quad (1.71)$$

Figure 1.18 illustrates the case of Lenz-Jensen interaction. You may note that even for rather small values of η there is a noticeable positive solid-gas difference.

1.6 Data

Numerous measurements have been performed aiming at equilibrium charges of ions penetrating through gaseous and solid materials. Experimental techniques have been described in classical reviews by Allison (1958) and Betz (1972) who focused on light and heavy ions, respectively. For a more recent review focusing on experimental methods, the reader is referred to Geissel et al. (2002).

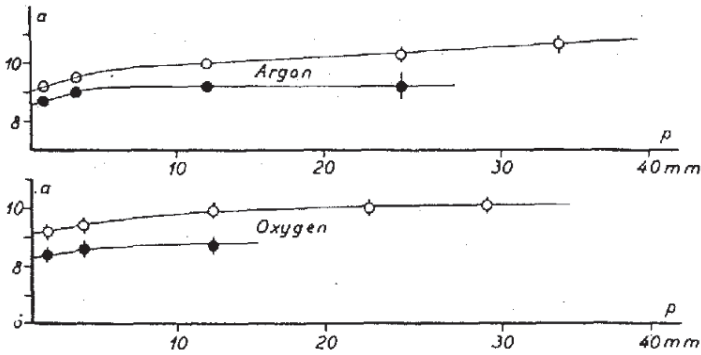


Fig. 1.19 Mean charges of light and heavy fission fragments penetrating through argon and oxygen vs. gas pressure, from Lassen (1951b)

1.6.1 Gas-Solid Difference

Pioneering measurements, performed by Lassen (1951b) by means of fission fragments, were mentioned in Sect. 1.1. In view of the limited range of accessible atomic numbers and beam energies, the most obvious variation to study appeared to be the influence of the medium. Measurements were performed on solids and gases, the latter as a function of gas pressure. Results were shown in Fig. 1.1.

Figure 1.19 shows equilibrium charges in gases vs. pressure, likewise from Lassen (1951b). A clear increase with gas pressure is seen. Here, as in Fig. 1.1, the charge increases with the electron density of the medium, pointing at a common origin. This will be discussed in Sect. 3.3.3.

1.6.2 Compilations

In view of the large number of projectile-target combinations of potential interest, much attention has been paid to scaling properties of the mean equilibrium charge $\langle q_1 \rangle$ in three-dimensional parameter space (Z_1, Z_2, v) . Guided by theoretical estimates of the type of (1.6), where properties of the target material do not enter at all, special efforts have been made to identify an adequate scaling variable of the type of $v/Z_1^{2/3}v_0$, while Z_2 -dependencies were most often treated as perturbations, except for gas-solid differences mentioned above.

Figure 1.20 shows average charge fractions for ions with Z_1 ranging from 16 to 92 for ions emerging from carbon foils (upper graph) and from gas targets (lower graph). Adopted scaling variables are $v/Z_1^{0.45}v_0$ according to Nikolaev and Dmitriev (1968) in the upper graph and $v/Z_1^{0.55}v_0$ in the lower graph (Betz, 1972). Noticeably higher values are observed in the upper graph over the entire velocity range covered, confirming the existence of a distinct gas-solid difference.

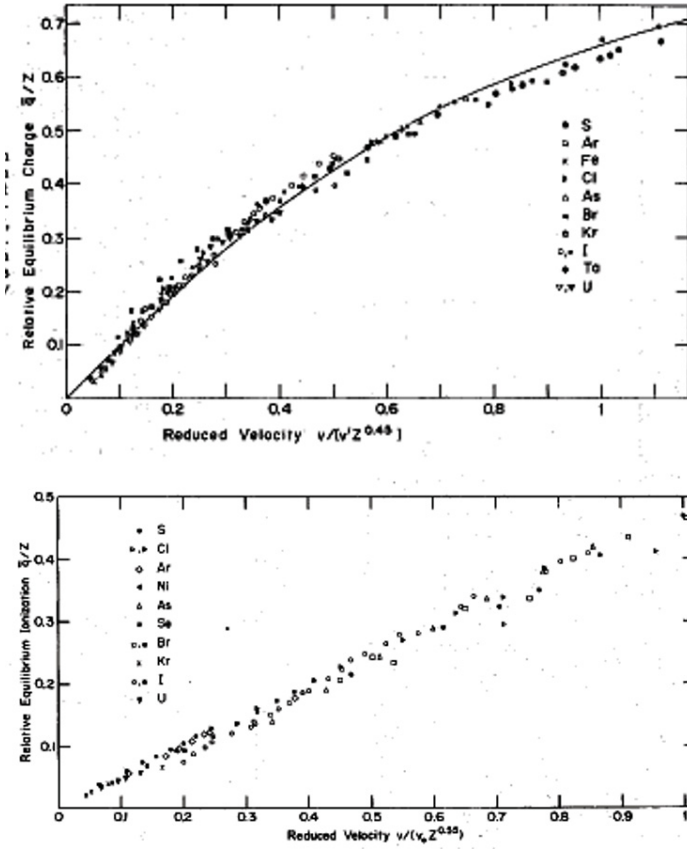


Fig. 1.20 Average charge fraction of sulphur to uranium ions vs. scaled velocity. Upper graph: Carbon foil. Velocity variable $v/Z_1^{0.45}v'$ with $v' = v_0/0.608$. Lower graph: Gas targets of N_2 , O_2 and air. Velocity variable $v/Z_1^{0.55}v_0$. From Betz (1972)

An extensive analysis of measured equilibrium charge fractions in carbon (Shima et al., 1982) has led to an empirical formula which has frequently been utilized in estimates also on other solid targets,

$$\frac{\langle q_1 \rangle}{Z_1} = 1 - e^{-1.25X + 0.32X^2 - 0.11X^3}; \quad X = 0.608v/Z_1^{0.45}v_0. \quad (1.72)$$

Comparison with (1.6) indicates a somewhat steeper slope in the low-velocity limit as well as a difference in the Z_1 -dependence.

More recently, Schiwietz and Grande (2001) proposed

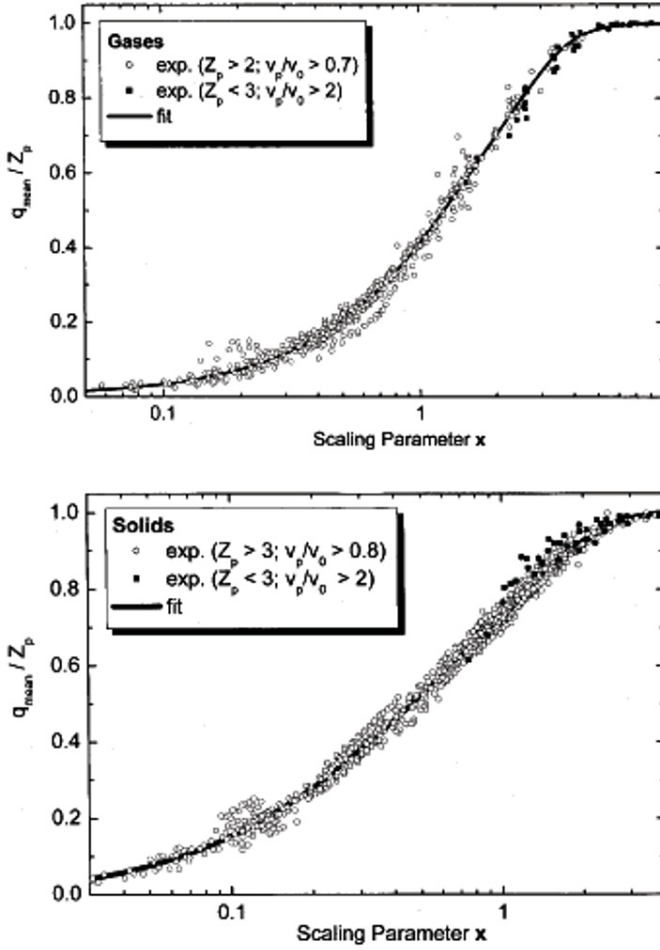


Fig. 1.21 Average charge fraction in gases (upper graph) and solids (lower graph) and empirical fits, (1.73) and (1.74) vs. scaled velocity. Z_p and v_p stand for Z_1 and v , respectively. From Schiwietz and Grande (2001)

$$\frac{\langle q_1 \rangle}{Z_1} = \frac{x^6 + 376x}{x^6 + 690x - 1206x^{0.5} + 1428}$$

$$x = \left(\frac{\eta}{Z_2^{0.017\eta - 0.03}} \right)^{1 + 0.4/Z_1} \quad (1.73)$$

for gas targets and

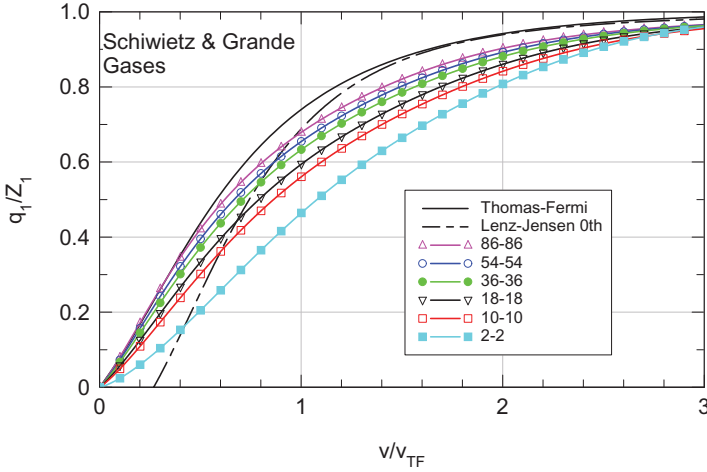


Fig. 1.22 Average charge fraction vs. speed according to Schiwietz and Grande (2001) for gases, plotted in Thomas-Fermi units. $Z_1 = Z_2$. Also included is the Thomas-Fermi curve from Fig. 1.9 and the zero-order Lenz-Jensen curve from Fig. 1.10.

$$\frac{\langle q_1 \rangle}{Z_1} = \frac{x^4 + 12x}{x^4 + 10.37x + 0.3x^{0.5} + 6 + 0.07/x}$$

$$x = \left(\frac{\eta}{1.68 Z_2^{0.019} \eta} \right)^{1+1.8/Z_1} \quad (1.74)$$

for solids with

$$\eta = \frac{v}{Z_1^{0.52} v_0}. \quad (1.75)$$

Here, the approach to complete ionization is asserted to be power-like rather than exponential. At low velocities, $\langle q_1 \rangle$ is asserted to be $\propto v^{1+0.4/Z_1}$ for gases and $\propto v^{2+3.6/Z_1}$ for solids.

Figure 1.21 gives an impression both of the quality of the scaling and the accuracy of the fit. Clearly, these fitting formulae are entirely empirical, and deviations from adopted scaling properties may well be systematic. On the other hand, rough estimates of equilibrium charge states are possible for systems where measurements are unavailable.

Figure 1.22 shows the curve from Fig. 1.21 plotted in Thomas-Fermi units. It is seen that the curve denoted ‘Thomas-Fermi’, taken from Fig. 1.9, lies consistently above the empirical interpolation, although the difference gets less pronounced with increasing atomic number. The Lenz-Jensen curve from Fig. 1.10 represents a reasonable average behaviour at low speed but approaches the TF curve at high speed.

Finally, Fig. 1.23 shows plots of (1.74) and (1.73) in Thomas-Fermi units. The gas-solid difference clearly emerges from these graphs, as well as the near-independence of the mean equilibrium charge on the atomic number of the stopping

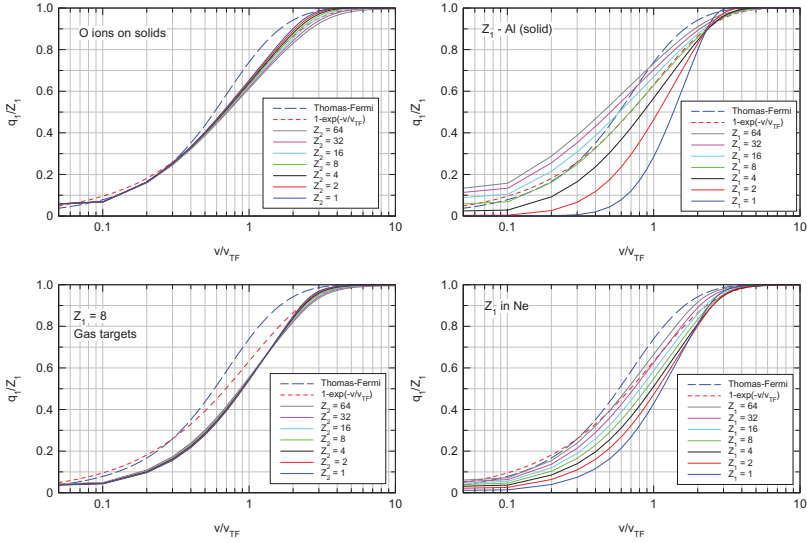


Fig. 1.23 Equilibrium charges according to Schiwietz and Grande (2001) plotted in Thomas-Fermi units

material. Conversely, deviations from v/v_{TF} scaling are pronounced, albeit mostly so for small Z_2 , where the Thomas-Fermi model cannot be expected to be valid.

You may have noticed that none of the scaling relations mentioned so far takes into account shell effects such as the plateaus seen in Figs. 1.3 and 1.7.

1.7 Discussion and Outlook

The prime message of this chapter is that ions in charge equilibrium experience considerable screening for $v \lesssim v_{TF}$ or

$$E \lesssim 0.025 Z_1^{4/3} \text{ MeV/u}, \quad (1.76)$$

and that the K shell can only be expected to be stripped for $v \gtrsim Z_1 v_0$ or

$$E \gtrsim 0.025 Z_1^2 \text{ MeV/u}. \quad (1.77)$$

Theoretical estimates presented in this chapter refer mostly to penetration through gas targets. The energy criterion has been dominating, mostly because it can be formulated quantitatively. Its main weakness is the lack of a statement on the time or pathlength required to reach charge equilibrium. Moreover, it does not say anything about the width of the charge-state spectrum. Thomas-Fermi estimates tend to predict higher equilibrium charges than measured.

Determining equilibration distances and charge-state populations requires explicit knowledge of the kinetics of charge exchange, as expressed by cross sections or transition amplitudes and appropriate statistical tools. This will be the subject of the following two chapters.

The observation of the gas-solid difference in the charge state and the ongoing controversy about its origin has, until a few years ago, been a considerable challenge to theoreticians. We shall come back to this repeatedly.

Both the very definition of the charge state of an atom moving in a medium and the validity of procedures to estimate transition probabilities or amplitudes have been the subject of lively discussion. I shall not go into details here but mainly mention a few points of interest and supply pertinent references.

From an experimental point of view, there are two obvious ways to approach the problem, observation of processes accompanying the emerging ion, and in situ analysis of the penetrating ion. The first option is related primarily to electron emission, the second to X-ray emission.

The first aspect has been discussed in Sect. 1.5.3. Bound states of swift protons moving through a solid material have been a subject of lively discussion. For a recent review you are referred to Arista (2006). Several theoretical predictions were based on the Fermi gas model described in Chap. 5, Vol. 1, but even within that framework, predictions varied from 0 to 2 permitted charge states (Brandt, 1975, Cross, 1977, Peñalba et al., 1992). Arista's conclusion appears to be close to the view of Cross (1977) who considered the coupling between the ion and the electron gas to be weak and, consequently, considered the charge-state evolution as a sequence of capture and loss processes much like in a gas.

As to the second aspect, in situ observation of charge states in solids is possible by X-ray spectrometry. Energies of inner-shell electrons are shifted according to the charge state. This *satellite* structure may be observed in precision measurements and thus may provide information about charge fractions of penetrating ions (Knudson et al., 1974). These experiments are difficult both because of the smallness of the shifts and the interference with the Doppler effect.

Measurements of this type appear most promising for heavy ions at very high velocities, where ions are highly charged and K X-ray levels shifted considerably. Results obtained with 11.4 MeV Ca ions by Rosmej et al. (2005) indicate a reasonable agreement between charge states deduced from x-ray spectra and those measured by magnetic deflection of ions after emergence from the foil.

1.8 Appendix

1.8.1 Exchange Energy in the Thomas-Fermi Equation

This appendix presents a brief derivation of the exchange term, (1.90).

Consider first a 2-electron system, where, in an individual-particle description, two stationary states 1 and 2 are occupied. Write the wave function $\Psi(x_1, x_2)$ in the form

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} [u_1(x_1)u_2(x_2) - u_2(x_1)u_1(x_2)], \quad (1.78)$$

where x stands for both space and spin variables. The Coulomb interaction energy is given by

$$E_{\text{Coulomb}} = \iint dx_1 dx_2 \Psi(x_1, x_2)^* \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \Psi(x_1, x_2). \quad (1.79)$$

Since e^2/r_{12} does not depend on the spin, E_{Coulomb} is nonvanishing only when the two states 1 and 2 have identical spin. We can, therefore, replace x by $\mathbf{r}$ and write

$$E_{\text{Coulomb}} = e^2 \iint d^3\mathbf{r}_1 d^3\mathbf{r}_2 \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} + E_{\text{exch}}, \quad (1.80)$$

where

$$E_{\text{exch}} = - \iint d^3\mathbf{r}_1 d^3\mathbf{r}_2 \frac{u_1^*(\mathbf{r}_1)u_2^*(\mathbf{r}_2)u_2(\mathbf{r}_1)u_1(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1.81)$$

where the first term represents the classical Coulomb interaction energy. We evaluate the exchange term $E_{\text{Coulomb}}^{\text{exch}}$ for free electrons with

$$u_j(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}_j \cdot \mathbf{r}}, \quad (1.82)$$

where Ω represents the volume of a large box. With this, the Coulomb potential has the expansion

$$\frac{e^2}{r} = \sum_{\mathbf{q}} \frac{4\pi e^2}{\Omega q^2} e^{i\mathbf{q} \cdot \mathbf{r}}. \quad (1.83)$$

Carrying out the above integral you will find

$$E_{\text{Coulomb}}^{\text{exch}} = - \frac{4\pi e^2}{\Omega (\mathbf{k}_1 - \mathbf{k}_2)^2}. \quad (1.84)$$

Now, consider a Fermi gas characterized by a density ρ or a Fermi wave number k_F . The total exchange energy is then given by the integral

$$\mathcal{E}_{\text{exch}} = - \left(\frac{\Omega}{(2\pi)^3} \right)^2 \iint d^3\mathbf{k}_1 d^3\mathbf{k}_2 \frac{4\pi e^2}{\Omega (\mathbf{k}_1 - \mathbf{k}_2)^2}. \quad (1.85)$$

If you are willing to solve Problem 1.4, you will find that

$$\mathcal{E}_{\text{exch}} = \frac{e^2 \Omega k_F^4}{4\pi^3}. \quad (1.86)$$

With

$$k_F^3 = 3\pi^2 \rho \quad (1.87)$$

you find the energy density

$$\frac{\mathcal{E}}{\Omega} = \kappa_a \rho^{4/3} \quad (1.88)$$

with

$$\kappa_a = \frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} e^2 \quad (1.89)$$

in the notation of Gombas (1949).

1.8.2 Thomas-Fermi-Dirac Theory

Following Gombas (1949), we take into account the exchange contribution (Dirac, 1930), which adds a term

$$E^{\text{exch}} = -\kappa_a \int d^3\mathbf{r} \rho(\mathbf{r})^{4/3} \quad (1.90)$$

with

$$\kappa_a = \frac{3^{4/3}}{4\pi^{1/3}} e^2 \quad (1.91)$$

to (1.13).

Carrying out the argument described in Sects. 1.4.1 and 1.4.2, you will obtain an additional term $-4(\kappa_a/3)\rho(\mathbf{r})^{1/3}$ to (1.21) which leads to

$$\rho(\mathbf{r}) = \sigma_0 \left(\tau_0 + \sqrt{\tau_0^2 + \phi(\mathbf{r}) - \phi_0} \right)^3 \quad (1.92)$$

with

$$\tau_0 = \sqrt{\frac{e}{2\pi^2 a_0}}. \quad (1.93)$$

Applying Poisson's formula you arrive at the Thomas-Fermi-Dirac equation

$$\nabla^2 (\phi(\mathbf{r}) - \phi_0 + \tau_0^2) = 4\pi\sigma_0 e \left(\tau_0 + \sqrt{\tau_0^2 + \phi(\mathbf{r}) - \phi_0} \right)^3 \quad (1.94)$$

or, in Thomas-Fermi units,

$$g''(\xi) = \xi \left[\sqrt{\frac{g(\xi)}{\xi}} + \beta_0 \right]^3 \quad (1.95)$$

with

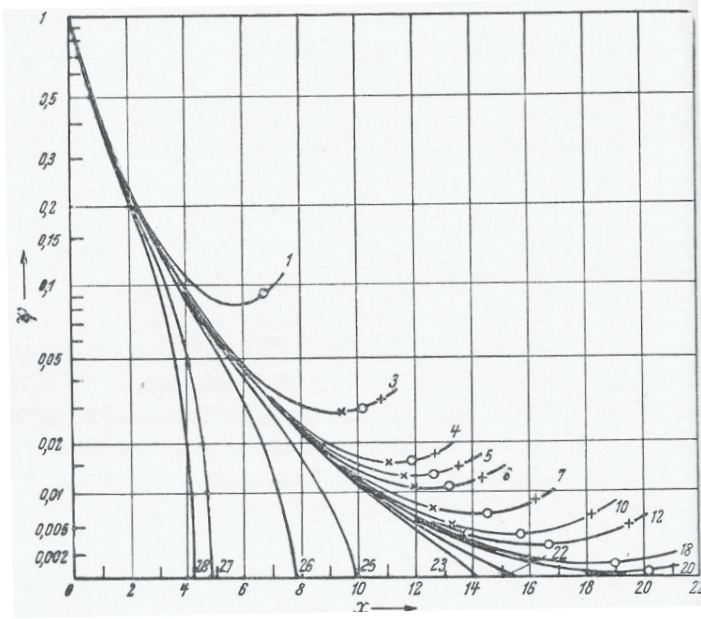


Fig. 1.24 Same as Fig. 1.8 for solutions of the Thomas-Fermi-Dirac equation. $Z_1 = 54$. From Gombas (1949)

$$\beta_0 = \tau_0 \sqrt{a/Z_1 e} = \frac{0.2118}{Z_1^{2/3}}, \quad (1.96)$$

$\xi = r/a$, and

$$\phi(r) + \tau_0^2 - \phi_0 = \frac{Z_1 e}{r} g(\xi). \quad (1.97)$$

So far, this derivation follows Gombas (1949), except again that the constant $\phi_0 = mv^2/2e$ is predefined, while the number N_1 of electrons on the projectile is free and follows from the charge density $\rho(\mathbf{r})$.

However, from (1.92) and Fig. 1.24 you may note that the charge density does not approach zero. Since the number of electrons must be finite, there must be a certain radius r_0 where $\rho(\mathbf{r})$ is truncated. Determining this radius is part of the minimizing procedure, as recognized by Jensen (1934, 1935). The present evaluation is slightly different, since there are no boundary conditions, but the result is identical with Jensen's.

Writing the total energy as

$$\begin{aligned} \mathcal{E}(N_1) = & \frac{1}{2} M_1 v^2 + \kappa_k \int d^3 \mathbf{r} \rho(\mathbf{r})^{5/3} - \kappa_a \int d^3 \mathbf{r} \rho(\mathbf{r})^{1/3} - Z_1 e^2 \int d^3 \mathbf{r} \frac{\rho(\mathbf{r})}{r} \\ & + \frac{e^2}{2} \int d^3 \mathbf{r} d^3 \mathbf{r}' \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{2} m v^2 \int d^3 \mathbf{r} \rho(\mathbf{r}), \quad (1.98) \end{aligned}$$

we minimize the energy with respect to r_0 ,

$$\frac{dE}{dr_0} = 4\pi r_0^2 \left(\kappa_k \rho(r_0)^{5/3} - \kappa_a \rho(r_0)^{4/3} - \frac{Z_1 e^2}{r} \rho(r_0) + \rho(r_0) e^2 \int_{r' < r_0} d^3 r' \frac{\rho(r')}{|\mathbf{r} - \mathbf{r}'|} \Big|_{r=r_0} + \frac{mv^2}{2} \rho(r_0) \right) = 0. \quad (1.99)$$

Noting that the third, fourth and fifth term in the brackets may be written as $-e\rho(r_0)[\phi(r_0) - \phi_0]$, and inserting $\phi(r_0) - \phi_0$ from (1.92) you end up with

$$\frac{dE}{dr_0} = 4\pi r_0^2 \rho(r_0) \left[\kappa_k \rho(r_0)^{2/3} - \kappa_a \rho(r_0)^{1/3} + 2e\tau_0 \left(\frac{\rho(r_0)}{\sigma_0} \right)^{1/3} - e \left(\frac{\rho(r_0)}{\sigma_0} \right)^{2/3} \right] \quad (1.100)$$

or

$$\frac{dE}{dr_0} = 4\pi r_0^2 \rho(r_0) \left[-\frac{2}{3} \kappa_k \rho(r_0)^{2/3} + \frac{1}{3} \kappa_a \rho(r_0)^{1/3} \right]. \quad (1.101)$$

Setting $dE/dr_0 = 0$ leads to

$$\rho(r_0) = \left(\frac{\kappa_a}{2\kappa_k} \right)^3 = \frac{0.002127}{a_0^3}. \quad (1.102)$$

This result is identical with the one quoted by Gombas (1949), although the derivation is simpler: For a fixed number N_1 of electrons, $\rho(r)$ and r_0 cannot be varied independently. Therefore, in the derivation of Gombas (1949) also a derivative $d\rho(r)/dr_0$ needs to be considered.

For the standard Thomas-Fermi model, where κ_a is ignored, we find $\rho(r_0) = 0$, in agreement with (1.34) in Sect. 1.4.2. For the Thomas-Fermi-Dirac model, on the other hand, the electron density at the edge has a fixed nonvanishing value, (1.102), independent of atomic number and charge state.

The number N_1 of electrons on the projectile is found from

$$N_1 = \int d^3 r \rho(r) = Z_1 \int_0^{\xi_0} d\xi \xi g''(\xi) = Z_1 [\xi_0 g'(\xi_0) - g(\xi_0) + 1] \quad (1.103)$$

or

$$q_1 = Z_1 - N_1 = Z_1 [g(\xi_0) - \xi_0 g'(\xi_0)]. \quad (1.104)$$

A major benefit of the straight Thomas-Fermi model is the universal dependence of the charge density on r/a_{TF} . This feature is no longer present in the Thomas-Fermi-Dirac model, where an explicit dependence on Z_1 enters via the term β_0 in (1.95). This, in addition to the abrupt fall-off to zero at r_0 , may well generate some doubt

as to whether including electron exchange in the theory is an overall improvement of the scheme. I shall touch this aspect once more in the next section.

Problems

1.1. Derive (1.29) and (1.30) from (1.18), (1.27) and (1.28).

1.2. Show that (1.31) approaches the solution

$$g(\xi) \sim 144/\xi^3 \quad (1.105)$$

for large ξ .

1.3. Compare the behaviour of $\rho(r)$ at small r for the exact solution of the Thomas-Fermi equation with the behaviour of the ansatz by Lenz and Jensen.

1.4. Derive (1.86) from (1.85). Hint: The straightforward but a bit cumbersome way is by introducing spherical coordinates and carrying out the angular integrations first. A more elegant procedure is making use of the Fourier transform of the Coulomb potential.

1.5. Show that, if (1.50) and (1.51) are valid, the equilibrium charge behaves as $\propto v^2$ at low projectile speed.

1.6. Try to reproduce the curves shown in Fig. 1.10.

1.7. Make an estimate of the expected difference between charge ratios for light and heavy fission fragments shown in Fig. 1.1 on the basis of (1.6).

1.8. Look up an element representative for heavy fission fragments and its representative energy, and find the gas-solid difference from (1.73) and (1.74). Compare this with Fig. 1.1.

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