Theory of Effective Charge and Stopping Power of Heavy Ions*

Stewart D. Bloom
Department of Applied Science, University of California, Davis, California 95616, and the Lawrence Radiation Laboratory, Livermore, California 94550

and

George D. Sauter
Department of Applied Science, University of California, Davis, California 95616,
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The Knipp-Teller theory of stopping power for heavy ions is reviewed and revised. The basic idea of using the Thomas-Fermi theory to describe the electron charge around the moving ion is retained. The major alteration which is introduced is in relating the degree of ionization to the velocity of the ion. The zero-order term of the resulting theory comes within 10% or so of predicting observed mean electronic stopping powers for ions with $z>6$ and $\epsilon/z^{4/3}>0.002$, where z is the atomic number of the ion and ϵ its kinetic energy in million electron volts per atomic mass unit.

With the advent of the newest medium energy accelerators (up to ≈150 MeV) and the enormous concomitant improvement in detection techniques of the last decade, there has come a considerable resurgence of interest in the physics of the stopping power of media for the various ions these machines produce.[1] In particular there has been a very active revival of the effective-charge theory of the electronic stopping of media for heavy ions. This theory was first proposed by Knipp and Teller[2] in 1941; it has not really been well tested until the last several years. As we shall explicitly show, and as is now generally realized, the qualitative aspects of this theory are already well substantiated.[1] We shall further show that a corrected version of this theory quantitatively predicts the observed (mean) electronic stopping power within about 10% or better for essentially all ions, except the very lightest such as He and possibly C, in any medium and over an energy range of 3 decades. We begin with a brief review of the main elements of the theory. This is followed by our amended version of the theory and its results.

The two basic assumptions which are made in the theory can be most easily stated as follows:

(a) The mean electronic stopping power S_e for any heavy ion of mass m and atomic number z can be expressed as the product of two factors:

$$S_e=(\gamma^2z^2)(S_{e0}), \tag{1}$$

where S_{e0} is defined as the stopping power of a bare proton with the same value of ϵ, the energy in units of million electron volts per atomic mass unit, as the heavy ion. γ^2, the effective charge parameter, is a correction factor $\geqslant 0$ and $\leqslant 1$ which is independent of the medium being traversed. (b) γ^2 should be functionally dependent only on the argument $\epsilon/z^{4/3}$.

Assumption (a) follows from first-order perturbation theory. Assumption (b) is based on the viral theorem and similarity transformations in the size and charge of the ion.[3] Both assumptions are known to be only approximately correct. In a more detailed approach, Lindhard, Scharff, and Schiott[4] have derived a formula for S_e which predicts a dependence on Z, the atomic number of the medium, for the energy region $\epsilon/z^{4/3}$ <0.025 and $z>10$, such that the stopping power per medium electron decreases with increasing Z at fixed $\epsilon/z^{4/3}$. Experimental evidence tends to support this theory,[1] which evidently contradicts (a). Also, the recent work of Betz and Grodzins[5,6] and other work cited in these papers show that there is some dependence of the charge state of heavy ions on both Z and the state of condensation of the medium. Of course all this work has been necessarily limited to observing the charge states of heavy ions emerging from the medium rather than in it, and also this dependence has been observed only at rather low values of $\epsilon/z^{4/3}$ ($\lesssim 0.003$). However it still implies some degree of violation of assumption (b) as well as (a). Nonetheless, the degree of breakdown of neither assumption (a) nor (b) destroys the basic correctness of Eq. (1), as we shall show.

Assumption (b) at first glance appears rather general and indeed its implementation requires more detailed models for the electron-loss process. In particular, Knipp and Teller used the Thomas-Fermi (TF) model to describe the ion and then calculated the average electronic energy $\langle T_e\rangle$ as a function of γ, the effective charge parameter. They then assumed that the electronic velocity v_e corresponding to $\langle T_e\rangle$ was proportional to v, the velocity of the heavy ion, taking the constant of proportionality k from the experimental data available at that time. In our theory we adopted the approach that it is more realistic to assume that the ionization energy of the most weakly bound electron still clinging to the ion should equal the maximum kinetic energy transferable to it by the electrons in the medium being traversed. Assuming that the medium electrons can be regarded as free, this then leads to the condition $v_f = v$, where v_f is the velocity of the last bound electron. Of course experimental values for the ionization energy of ions in various states of charge are known and could be used directly. However what we need is a *statistical* value for v_f which, by averaging, takes out the effect of large variations in the vicinity of the closure of atomic shells. Thus the Thomas-Fermi-Dirac (TFD) theory with corrections for correlation effects[7] would be the most accurate and appropriate one to use. The inclusion of exchange effects (i.e., the TFD theory) and the further inclusion of correlation effects are large corrections and cannot be ignored.[7] Both corrections can be done statistically. However, even the TF theory does not yield a result such that γ is a function of only the variable $\epsilon/z^{4/3}$, if one considers specifically the ionization energy of the last bound electron. Indeed it is possible to show that the proper statistical relationship is given by a power series of the following form:

$$v_f{}^2/z^{4/3} = \sum_{q=0}^{\infty} f_q(\gamma)/z^q, \tag{2}$$

where the function $f_q(\gamma)$ can be computed using the TFD theory with correlation corrections. [The derivation of Eq. (2) and the functions $f_q(\gamma)$ will be given in a more detailed paper later.] The equality $v_f = v$ leads immediately to

$$\epsilon/z^{4/3} = K\textstyle\sum_q f_q(\gamma)/z^q, \tag{3}$$

where K is the constant relating ϵ and v^2. It is clear that all the terms in Eq. (3) with $q \geq 1$ represent deviations from approximation (b). However, as we shall see, the experimental data suggest that the predominant term is the first one, $q = 0$, and in this paper we will consider only this term. We give (without derivation) the function $f_0(\gamma)$:

$$f_0(\gamma) = \lim_{z\to\infty} \frac{Q_n' - Q_{n-1}'}{z^{7/3}} \tag{4a}$$

which, using Eq. (2), gives

$$\epsilon/z^{4/3} = Kf_0(\gamma). \tag{4b}$$

Q_n' is the total binding energy for an atom of atomic number z and electronic charge $n \leq z$. The prime on Q_n' is meant to indicate that exchange and correlation corrections to the binding energy have been included. Both corrections are generally non-negligible, as may be seen from the rough relationship adopted for the present work:

$$Q_n' \approx 1.6 Q_n, \tag{5}$$

where Q_n is the uncorrected TF energy. The factor 1.6 is taken from the work of Gombas.[7] In the later paper a more exact treatment of the exchange and correlation corrections will be given. These corrections will depend on v_f (and hence ϵ) and also, like the higher-order terms in Eq. (2), on z, which implies a deviation from approximation (b).

The results of our calculations are shown by the solid-line plot in Fig. 1. An attempt has been made to put a sample of the vast amount of available experimental data on the figure which is representative of all the ions and all the media as well. In doing this we have drawn heavily on the tabulation by Northcliffe and Schilling.[1] For values of $\epsilon/z^{4/3} < 0.01$ we used fission-fragment data[8] and data for heavy ions in gases.[9] Theory and experiment for these data are too close to show on the figure but the agreement is essentially of the same character as for the higher energies. Figure 1 does show the earlier result of Knipp and Teller (Ref. 2) as well as a recent empirical fitting to the experimental data in the parameter $\epsilon/z^{4/3}$.[9] This last curve will be discussed a little later.

Several things are immediately clear from Fig. 1: First, from the experimental data alone we see that both assumptions (a) and (b) are well sustained. Second, the Knipp-Teller theory fails badly, a circumstance which cannot be altered by changing the constant K (see above). However, the agreement of the new theory with experiment is, in general, quite good, being within 5% or better of the mean of the experimental points for a fixed value of $\epsilon/z^{4/3}$ except in the region $0.1 < \epsilon/z^{4/3} < 0.2$, where is seems clear that the theory systematically overestimates $\gamma_{\exp}{}^2$ by as much as 10%.

Also shown in Fig. 1 is the semiempirical fitting to $\gamma_{\exp}{}^2$ made by Pierce and Blann[9] (dashed

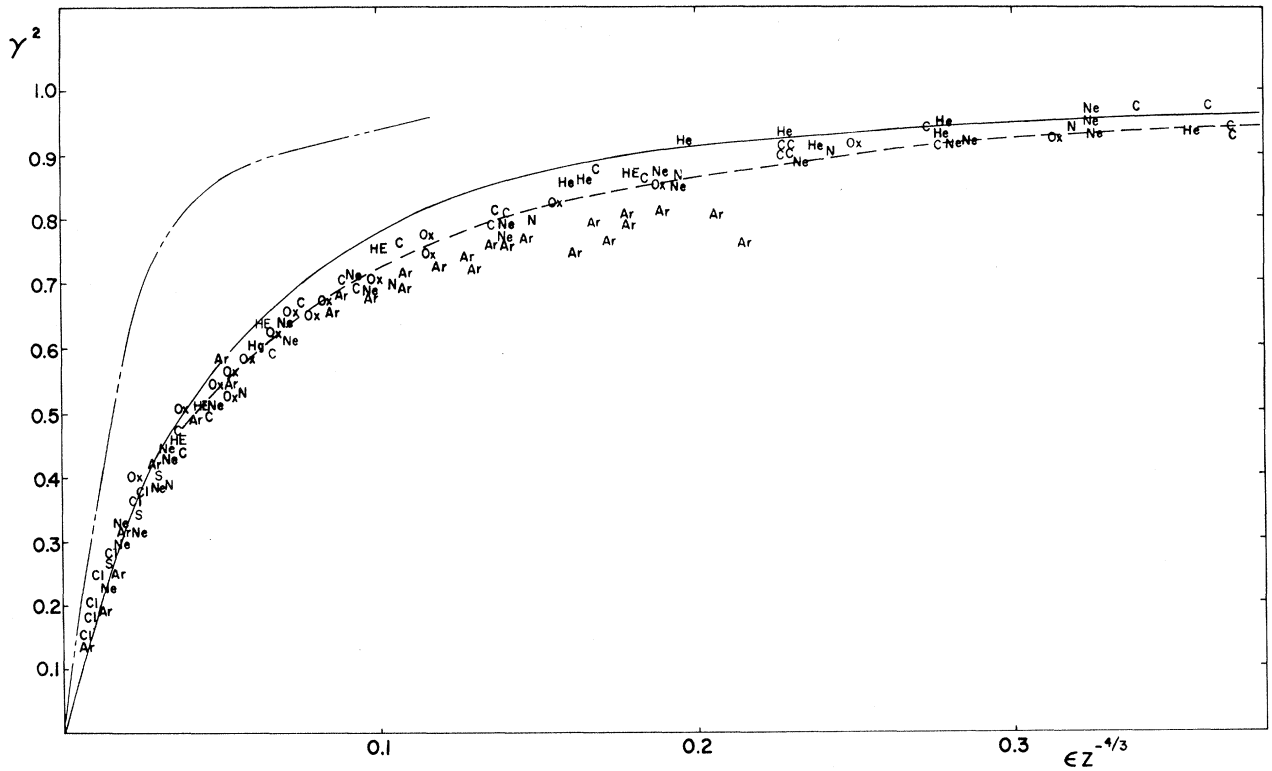

FIG. 1. γ^2, the square of the effective charge parameter, versus the energy parameter $\epsilon z^{-4/3}$, where ϵ is the ion energy in million electron volts per atomic mass unit and z is the ion atomic number. The dot-dashed curve was calculated according to the theory of Knipp and Teller (Ref. 2); the dashed curve is the semiempirical formula of Ref. 9 [see Eq. (6)]; the solid curve is the present theory. The experimental points are taken from the references quoted in the tabulation of Northcliffe and Schilling (Ref. 1). The symbols denoting the ions are standard except for the HE which stands for heavy ions in Mylar (see Ref. 9).

line). For $\epsilon > 0.3$ their formula for γ is

$$\gamma = 1 - \exp[-6.35(\epsilon/z^{4/3})^{1/2}]. \tag{6}$$

The restriction to $\epsilon > 0.3$ corresponds to energies such that the proton, whose stopping power is the basis of Eq. (1), is effectively bare. As can be seen from Fig. 1, Eq. (6) fits the data rather well. Its simplicity leads one to suspect that there may be a theoretical basis for the form of Eq. (6). Unfortunately, comparison of Eq. (6) with our theory [Eq. (4b)] is complicated by the fact that the Thomas-Fermi approach leads to expression of $\epsilon/z^{4/3}$ in terms of γ rather than vice versa. Thus for $\epsilon/z^{4/3} < 0.1$ we obtained the following form for $\epsilon/z^{4/3}$ as a consequence of studying the behavior of $f_0(\gamma)$ [see Eq. (4a)]:

$$\epsilon z^{-4/3} = a\gamma/(1-b\gamma)^2, \tag{7}$$

where a and b are adjustable constants with the limitation that b should be less than, but in the vicinity of, unity. The details concerning the derivation of Eq. (7) will be given in the later paper. The experimental data are best fitted using values $a = 0.0086$ and $b = 0.86$. In Fig. 2 we show $\epsilon/z^{4/3}$ as a function of γ using Eqs. (6) and (7), as well as an average of the experimental results shown in Fig. 1. As can be seen, both Eqs. (6) and (7) approximate the experimental curve very well except perhaps in the vicinity of $\gamma = 1$. At this point Eq. (6) becomes infinite, whereas Eq. (7) predicts complete ionization ($\gamma = 1$) at $\epsilon z^{-4/3} = 0.44$, a consequence of the fact that the Thomas-Fermi theory leads to a finite energy for total ionization. Of course Eq. (6) can be altered to make a similar prediction by adding another adjustable constant. However, even with the addition of such a constant, the inversion of Eq. (6) (so that $\epsilon z^{-4/3}$ is expressed as a function of γ) leads to a much more complicated expression than Eq. (7). Thus the similarity of the form of the two curves in Fig. 2 is almost certainly fortuitous.

To summarize, the Thomas-Fermi theory as used above provides a practical basis for pre-

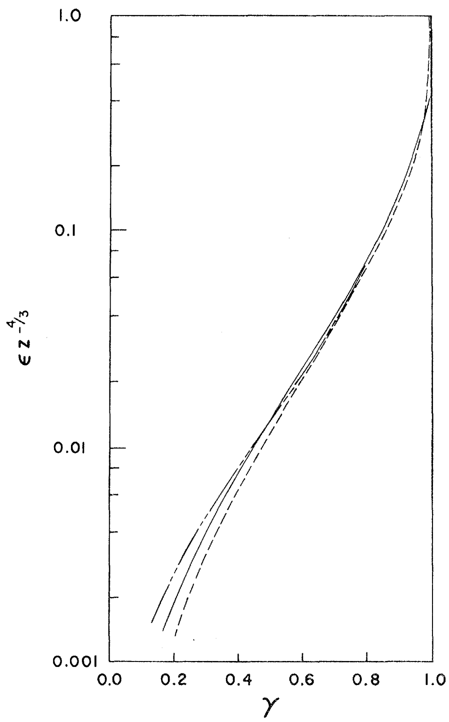

FIG. 2. Plots of the energy parameter, $\epsilon z^{-4/3}$, versus the effective charge parameter γ. The solid curve is based on an average of the experimental data shown in Fig. 1. The dashed curve is a replotting of the semiempirical curve of Ref. 9 [see Eq. (6) and the dashed curve of Fig. 1]. The dot-dashed curve is a semiempirical formula based on our Thomas-Fermi theory [see Eq. (7)]. Note that the Thomas-Fermi theory predicts total ionization ($\gamma=1$) at $\epsilon z^{-4/3}=0.44$.

dicting the mean electronic stopping power for all ions with $z>6$ and $\epsilon>0.3$, the latter limitation corresponding to the range over which S_{e0}, the stopping power for a bare proton, is known. The three main limitations of the theory are (1) the uncertainty of the correction for exchange and correlation effects, (2) the neglect of fluctuations, and (3) the breakdown of the statistical model for velocities in the vicinity of the electron velocities of the K and L shells. Techniques already exist for remedying (1),[3,7] and these will be used in the later paper. With regard to (2), it is important to emphasize that the approach outlined above is only a theory of electron stripping. A complete statistical theory should include mechanisms for capture and loss which would then lead to predictions of the fluctuation of γ, i.e., an effective charge distribution.[5,6] With regard to (3) we note the following: At very high energies ($\epsilon z^{-4/3}>0.3$) the ion will be almost totally ionized (see Fig. 1), so that the statistical theory will not be much in error in any case. In the region $v\approx ze^2/\hbar$, i.e., the velocity of the K-shell electron, present evidence[1,10] is that most appropriate parameter is ϵz^{-1}. This region corresponds to $0.08\lesssim\epsilon z^{-4/3}\lesssim 0.2$ for the ion data given in Fig. 1. Here the statistical theory will probably overestimate γ until v is well in excess of $ze^2/\hbar$. At lower energies, $\epsilon z^{-4/3}<0.1$, the statistical theory should be valid since distribution of the atomic electrons being stripped becomes more continuous. This qualitatively explains the deviations of the present theory from experiment as shown in Fig. 1. Thus, with the exchange and correlation corrections and z-dependent corrections properly taken into account, we should be able to assess quantitatively the relative roles of electron capture and loss and/or the limitations of the statistical model in predicting γ.

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