Inasmuch as s and f_2' are less than or equal to unity, approximations (2) and (3) are less restrictive than (1). The results for the population distribution agree with those obtained from the rate equations in first order when approximation (1) is also made.

The new features of this paper include explicit calculations of the internal energy, heat capacity, entropy, saturation parameter, and minimum entropy production of a three-level maser. The spontaneous emission and cross relaxation mechanisms introduced tend to reduce the value of the saturation parameter from its value given in terms of w_{ij} and W_{13} alone. Since w_{2123} is appreciable when $\nu_{21}-\nu_{32}$ is small, this cross relaxation mechanism has an interesting effect on the maser's internal energy and heat capacity as can be seen by an inspection of Eqs. (32)–(35) inclusive. As s goes from 0 to 1, the internal energy of a three level maser is increased by $(2Nh^2/9kT)(\nu_{21}^2+\nu_{21}\nu_{32}+\nu_{32}^2)$ whereas the associated heat capacity is decreased from its equilibrium value of $(2Nh^2/9kT^2)(\nu_{21}^2+\nu_{21}\nu_{32}+\nu_{32}^2)$ to zero.

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Energy Dissipation by Ions in the kev Region

J. Lindhard
Institute of Physics, University of Aarhus, Aarhus, Denmark

AND

M. Scharff*
Institute for Theoretical Physics, University of Copenhagen, Copenhagen, Denmark

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At low energies ionic collisions with atoms are largely elastic. Simple theoretical approximations to scattering cross sections, ranges and straggling are derived for power potentials, showing that the scattering is peaked in the forward direction rather than isotropic. Using an approximate universal potential of Thomas-Fermi type a natural measure of range, ρ, and of energy, ϵ, is obtained for all ions in all substances. The corresponding range-energy curve is computed.

At higher ion energies the electronic excitation becomes increasingly important. An approximate formula is given for the electronic stopping contribution, increasing proportional to ion velocity at low and moderate velocities. These results are applied in the interpretation of a few isotope effects, observed in range measurements.

FOR ions with velocity v comparable to or less than $v_0=e^2/\hbar$, an interesting competition appears between loss of energy to electrons and loss of energy to atomic recoils, corresponding to stopping cross sections per atom S_ϵ and S_ν. Quantities of importance to this competition are S_ϵ and S_ν, combined with some averages over the differential cross section $d\sigma_\nu$ for scattering of the ion by a recoiling atom. The present discussion of the velocity region $v\lesssim v_0$ is intended as a step toward a quantitative treatment of the processes involved.

At first we shall disregard energy loss to electrons and discuss atomic recoils only. Bohr[1] introduced the assumption that S_ν is nearly a constant in a considerable velocity interval at low velocities, and used arguments of the Thomas-Fermi type in order to give a comprehensive description. In fact, the Thomas-Fermi treatment gives an important simplification and a fair accuracy, at energies large compared to the Rydberg unit.

The scattering problem in nearly elastic collisions between atoms and ions at low velocities can be treated by classical mechanics. It follows from dimensional arguments that the potential must behave as r^{-2} if S_ν is independent of velocity. The scattering in this potential is very closely given by the useful formula

$$d\sigma_\nu=(S_\nu/2T_m^{\frac{1}{2}})\ (dT/T^{\frac{3}{2}}), \tag{1}$$

where $T_m=2M_1^2M_2v^2/(M_1+M_2)^2$ is the maximum value of the energy transfer T. The scattering cross section (1) has a large probability for small angular deflections, and is similar to the Rutherford scattering rather than to the isotropic scattering of hard-sphere collisions. Assume that the potential is $V=\xi_\nu Z_1Z_2e^2a/2r^2$, with the parameter a given by

$$a=(\hbar^2/me^2)\times 0.8853(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}})^{-\frac{1}{2}}, \tag{2}$$

and therefore of similar type to the Thomas-Fermi unit of length. We then obtain the formula

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* Deceased.

[1] N. Bohr, Kgl. Danske Videnskab. Selskab, Mat.—fys. Medd. **18**, No. 8 (1948).

$$S_\nu=\int Td\sigma_\nu=\xi_\nu(\pi^2/2)e^2aZ_1Z_2[M_1/(M_1+M_2)]. \quad (3)$$

This expression is similar to that used by Bohr.[1] A reasonable value of the coefficient in the r^{-2} potential is[2] $\xi_\nu=2/(2.7183\times0.8853)$.

The average range is proportional to the energy, and from (1) the square of the straggling in range is found to be[2]

$$\langle(\Delta R)^2\rangle_{\mathrm{av}}/\bar{R}^2=\alpha[M_1M_2/(M_1+M_2)^2], \quad \alpha=\tfrac{2}{3}, \quad (4)$$

which is half the value obtained by Bohr[1] assuming isotropic scattering.

The average range measured along the track, $\bar{R}$, is usually not the quantity observed experimentally. In fact, frequently the observed quantities are related to the average projected range, $\bar{R}_p$, which may be defined as follows. A particle starts inside a homogeneous medium from the origin in the direction of the x axis; the value of x for the end point is the projected range, and its average is the average projected range $\bar{R}_p$. From (1) we obtain

$$\bar{R}/\bar{R}_p=\frac{1}{4}\left[-1-3\mu+(5+\mu)\frac{1+\mu}{2\sqrt{\mu}}\arccos\frac{1-\mu}{1+\mu}\right] \cong 1+\tfrac{1}{3}\mu, \quad (5)$$

where $\mu=M_2/M_1$. As regards the straggling it may be noted that $\langle\Delta R_p{}^2\rangle_{\mathrm{av}}\approx\langle\Delta R^2\rangle_{\mathrm{av}}$.

The domain of validity of the above formulas can be described by the parameter $\epsilon=a/b$, where $b=2Z_1Z_2e^2/M_0v^2$ is the collision diameter. The formulas can be expected to hold when $\epsilon\lesssim1$, since all collisions must then take place at separations with screened field. The formulas (1) to (5) are only first-order approximations to the atomic scattering. Still, for many purposes they remain preferable to more accurate formulas because of their simplicity and comparative accuracy.

These simple considerations may be extended. We consider first the consequences of a power potential, proportional to $Z_1Z_2a^{n-1}/r^n$. Then, S_ν behaves as

$$a^{2-2/n}(Z_1Z_2)^{2/n}[M_1/(M_1+M_2)][M_2E/(M_1+M_2)]^{1-2/n},$$

and the differential cross section is

$$d\sigma_\nu=(1-1/n)(S_\nu/T_m{}^{1-1/n})dT/T^{1+1/n},$$

to a good approximation. It is interesting to observe that this $d\sigma_\nu$ leads to a square of relative straggling in range given by (4), with $\alpha=4(n-1)/n(2n-1)$. Thus, the straggling is rather insensitive to the power n, for $n\sim2$, and has a maximum, $\alpha_{\mathrm{max}}=0.69$. This result leads us to expect that (4) may be quite accurate also in cases where (1) and (3) do not apply, and that measurements of relative straggling in range normally give little information about the potential and the effective value of the important quantity n. This expectation is confirmed by more accurate computations of straggling.

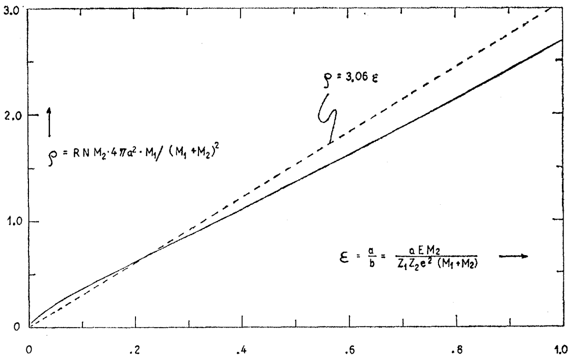

FIG. 1. The full-drawn curve is computed range as a function of energy in a ρ-ϵ plot, with neglect of energy loss to electrons. The increasing reduction in range due to energy loss to electrons will be of order of 20% for $\epsilon=1$.

The second extension is introduction of a potential energy of the type $V=Z_1Z_2e^2\varphi(r/a)/r$, where φ is a universal function, and a is given by (2). This assumption of similarity of the potential energy between any two atoms implies a natural measure of ion energy, $\epsilon=a/b$, and of particle range, $\rho=RNM_2\times4\pi a^2M_1/(M_1+M_2)^2$. It is thus informative to plot range-energy measurements in a ρ-ϵ plot, where a curve common to all ions and all substances should obtain to a first approximation. Of course, S_ϵ must be small, or properly corrected for. Due corrections should also be made for the type of range measured. For this purpose formulas like (1) and (5) may be adequate.

It turns out that a fair approximation to an adiabatic potential energy is achieved by putting $\varphi(r/a)=\varphi_0(r/a)$, i.e. the Fermi function belonging to one neutral atom. [The Fermi function is superior to an exponential screening like $\exp(-r/a)$.] We have computed the corresponding range curve, as shown in Fig. 1. For comparison is shown also the straight line $\rho=3.06\epsilon$ which would follow from (3) with the standard value of ξ_ν. Range measurements[2-7] are not plotted on the figure, but they seem in fair agreement with the computed curve.

Loss of energy to electrons may now be included. Several arguments show that S_ϵ is nearly proportional to v at low velocities, i.e., for v small compared to v', where $v'\sim Z_1^{2/3}v_0$. A simple way of showing the proportionality to v is to note that at low velocities the energy loss becomes proportional to v for an atom moving through an electron gas of constant density.[8] The variation of S_ϵ with Z_1 and Z_2 may be discussed using a

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Thomas-Fermi treatment. To a first approximation we find

$$S_\epsilon = \xi_\epsilon \times 8\pi e^2 a_0 (Z_1 Z_2/Z)(v/v_0), \tag{6}$$

with $Z=(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}})^{\frac{3}{2}}$, and where ξ_ϵ is of order of 1–2, but may vary with Z_1 approximately as $\xi_\epsilon \approx Z_1^{\frac{1}{6}}$. The dependence of S_ϵ on Z_1 and Z_2 in (6) is an expedient to get simple estimates. Empirically, the formula (6) is not far in error. Of course, for $v \gtrsim v'$ the formula (6) no longer holds, and the stopping cross section will reach a maximum and decrease at higher velocities.

We observe that (6) and (3) become equal at some energy E_c. If we put $Z_1=Z_2$ we find $E_c=Z_2^{\frac{4}{3}}A_2(\xi_\nu/\xi_\epsilon)^2 \times 750$ ev $\approx Z_2 A_2 \times 500$ ev, i.e., $\epsilon_c \approx 6A_2 Z_2^{-\frac{4}{3}}$, but already somewhat below this energy S_ν has fallen below (3) and $d\sigma_\nu$ approached the Rutherford scattering cross section. In many measurements, then, one observes a nearly constant S at energies about E_c. However, it is composed of a decreasing S_ν and an increasing S_ϵ. This effect will show up, e.g., as a reduction of relative straggling in range, since the straggling from collisions with electrons is negligible.

An instructive application of the above scattering formulas for power potentials is the hydrogen-deuterium isotope effect. In fact, when a heavy ion moves through a light substance ($M_1 \gg M_2$), S_ν varies with M_2 as $M_2^{1-2/n}$. To S_ν should be added S_ϵ which is independent of M_2; accordingly, for $n=2$ the stopping is independent of M_2. For $n-2$ positive, the heavier isotope will give the larger stopping, and vice versa. This result leads to an interpretation of range differences observed in hydrogen and deuterium. For large ϵ the value of n is between 1 and 2, and therefore $R_D > R_H$.[4,9] For small ϵ we expect n to increase beyond 2, so that $R_D < R_H$.[5]

Another interesting isotope effect is observed when M_1 is varied for fixed Z_1. Davies[6] has measured the shift in projected range between Na^{22} and Na^{24} of energy 24 kev in Al. Here, we expect a small energy loss to electrons, so that Eqs. (1), (3), and (5) are approximately valid. The results of Davies are in fair accord with Eq. (5).

More extensive publications are forthcoming on these and related subjects. Several of the above results were obtained five years ago, following discussions with Dr. R. B. Leachman on his observations of range distributions.[2] We are much indebted to Dr. Leachman for these discussions. We are grateful to Dr. J. M. Alexander, Dr. B. G. Harvey, and Dr. N. O. Lassen for communication of experimental observations prior to publication.

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Variational Method for Scattering Length

Takashi Ohmura*
Department of Physics, Washington University, St. Louis, Missouri

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The properties of the scattering length obtained by Kohn's method, which is one of Hulthén's variational methods, are studied by assuming a linear trial function with n adjustable parameters. The scattering length $A^{(n)}$ decreases monotonically as the number of adjustable parameters n increases, if there is no bound state in the system. This conclusion essentially comes from the upper bound theorem of Spruch and Rosenberg. When the system has m bound states, the scattering length increases in value only m times, and otherwise decreases monotonically. Therefore, after one verifies the presence of m increases, the calculated value is certain to give an upper bound on the scattering length. The connection between the result above and the condition of Rosenberg, Spruch, and O'Malley is considered. In the Appendix comparison is made of the scattering length $A^{(n)}$ obtained by Hulthén's original method and Kohn's method when m bound states exist in general.

I. INTRODUCTION AND SUMMARY

SPRUCH and Rosenberg[1] have recently proved that the Kohn method, which is one of the Hulthén variational methods, gives an upper bound on the scattering length if there is no bound state in the system. Rosenberg, Spruch, and O'Malley[2] have extended the theorem to the case where m bound states exist and showed that the calculated scattering length also gives an upper bound if the trial function is chosen so flexible that m approximate orthogonal-wave functions for the bound states with negative-energy expectation values can be formed by a linear combination of the terms involved in the trial function. The upper-bound theorem is useful because we can judge which is the better calculation and how the result is improved.

The purpose of the present note is to study the nature of convergence in the variational calculation with a

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* Now at Department of Physics, University of Tokyo, Tokyo, Japan.

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