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Inelastic Collisions and the Molière Theory of Multiple Scattering*

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The effect of inelastic collisions is often introduced in the Molière theory by replacing Z^2 with $Z(Z+1)$. It is pointed out that this procedure relies on the implied incorrect assumption that elastic and inelastic collisions have the same small-angle cut-off. Taking into account separately the cut-off of inelastic collisions, the Molière theory is shown to require the following modifications: (a) For incident electrons, replace Z^2 with $Z(Z+1)$ *and* increase the Molière b by $(Z+1)^{-1}\{\ln[0.160Z^{-\frac{2}{3}}(1+3.33Ze^2/h\nu)]-u_{\rm in}\}$, where $-u_{\rm in}$ is defined as an integral over the incoherent scattering function whose value is about 5. (b) For incident heavy particles, leave Z^2 unaltered but increase b by $Z^{-1}\{\ln[1130Z^{-4/3}(c^2/v^2-1)^{-1}]-u_{\rm in}-\frac{1}{2}v^2/c^2\}$.

1. INTRODUCTION

THE multiple scattering of charged particles traversing a material is treated by the Molière theory.[1,2] The scattering arises primarily from elastic collisions against the Coulomb field of atomic nuclei. Inelastic collisions with atomic electrons also contribute to multiple scattering, especially in light elements, but are disregarded, initially, in the Molière theory. To make allowance for inelastic collisions the squared nuclear charge Z^2 is often[2–4] replaced with the sum of the squares of the nuclear and electronic charges Z^2+Z. This procedure would be correct if the single scattering cross sections were given adequately by the Rutherford formula, i.e., were proportional to the squared charges of the colliding particles.

However, the actual cross sections depart at small angles from the Rutherford formula. The Rutherford rise to infinity is actually "cut off," and the cutoff differs for elastic and inelastic collisions[5] since it depends, respectively, on the density distribution of atomic electrons and on their binding. The binding effect is characterized for the inelastic collisions of particles, as well as of x-ray photons, by the "incoherent scattering function" S.[5]

The cut-off has a substantial influence on multiple scattering. Therefore, the replacement of Z^2 with $Z(Z+1)$ serves only to estimate the order of magnitude of the effect of inelastic collisions. (The same situation is encountered in bremsstrahlung and pair-production processes.) The present paper introduces inelastic collisions into the Molière theory *ab initio*.

Departures from the Rutherford formula are also encountered at large angles. For incident electrons these departures are comparatively minor, being due to exchange, spin, and relativity effects, and will be discussed briefly in Sec. 4. For inelastic collisions of incident heavy particles, large angle deflections are suppressed, by the requirements of momentum conservation; this effect causes the inelastic multiple scattering to be Gaussian rather than Molière-like (see Sec. 5).

2. SMALL-ANGLE EFFECTS FOR INCIDENT ELECTRONS

We deal with the Goudsmit-Saunderson form of the theory of multiple scattering, according to which the angular distribution of particles after a path length t is given by (39) of B53, namely[6]

$$f(t,\vartheta)=\sum_l(l+\tfrac{1}{2})P_l(\vartheta)\times\exp\left\{-Nt\int_0^\pi\sigma(\chi)\sin\chi d\chi[1-P_l(\chi)]\right\},\quad(1)$$

where $\sigma(\chi)$ represents the differential cross section for single scattering by an angle χ and the other symbols have their usual meaning. We separate the elastic and inelastic components of

$$\sigma(\chi)=\sigma_{\rm el}(\chi)+\sigma_{\rm inel}(\chi),\quad(2)$$

and set ourselves the task of comparing the contribution of $\sigma_{\rm inel}$ to the exponent of (1) with the contribution of $\sigma_{\rm el}$. For the purpose of this comparison $\sigma_{\rm el}$ will be taken, according to (44) and (10) of B53, in the form

$$Nt\sigma_{\rm el}(\chi)\sin\chi d\chi=2Z^2\bar{\chi}_c^2q(\chi)\sin\chi d\chi/4(1-\cos\chi)^2\quad(3)$$

$$\bar{\chi}_c^2=4\pi Nte^4z^2/p^2v^2,\quad(4)$$

where ze, p, and v are the charge, momentum, and velocity of the incident particle, $q(\chi)$ is an unspecified screening function, and $\bar{\chi}_c^2$ differs from the χ_c^2 of (10-B53) by the deletion of $Z(Z+1)$.

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[1] G. Molière, Z. Naturforsch. 3a, 78 (1948).
[2] H. A. Bethe, Phys. Rev. 89, 1256 (1953); this paper constitutes the point of departure of the present treatment and will be referred to as B53.
[3] L. A. Kulchitsky and G. D. Latyshev, Phys. Rev. 61, 254 (1942).
[4] Hanson, Lanzl, Lyman, and Scott, Phys. Rev. 84, 634 (1951).
[5] P. M. Morse, Physik. Z. 33, 443 (1932); see also, e.g., M. Pirenne, *Diffraction of X Rays and Electrons by Molecules* (Cambridge University Press, London, 1946), p. 54, p. 25 ff.

[6] The "detour factor" mentioned in B53 after Eq. (39) is comparatively unimportant. Arguments from which this factor can be estimated are presented by L. V. Spencer and C. H. Blanchard, this issue [Phys. Rev. 93, 114 (1953)], footnote 14.

For inelastic collisions we can similarly write[5,7]

$$Nt\sigma_{\mathrm{inel}}(\chi)\sin\chi d\chi=2Z\bar{\chi}_c^2S(v)\sin\chi d\chi/4(1-\cos\chi)^2, \quad (5)$$

where

$$v=0.333Z^{-\frac{1}{3}}(pa/\hbar)[2(1-\cos\chi)]^{\frac{1}{2}} \sim 0.333Z^{-\frac{1}{3}}(pa/\hbar)\chi \quad (6)$$

is a convenient dimensionless function of χ,[8] a is the Bohr radius, and $S(v)$ is the incoherent scattering function[5,8] which describes the small angle cutoff in (5) as $q(\chi)$ describes it in (3).

In the Molière theory, the small-angle cutoff is adequately characterized by a single parameter, the angle χ_a defined by (16-B53),

$$-\ln\chi_a=\lim_{k=\infty}\left[\int_0^k q(\chi)d\chi/\chi+\tfrac{1}{2}-\ln k\right]. \quad (7)$$

Similarly we define an inelastic cut-off angle χ_{in} by

$$-\ln\chi_{\mathrm{in}}=\lim_{k=\infty}\left[\int_0^k S(v)d\chi/\chi+\tfrac{1}{2}-\ln k\right]. \quad (8)$$

The values of χ_{in} and of χ_a will be compared in Sec. 3.

If the contribution of elastic collisions to the exponent of (1) is calculated according to the Molière theory, this contribution depends on χ_a through a term

$$\tfrac{1}{4}Z^2\bar{\chi}_c^2 l(l+1)\ln(\chi_a^{-2}), \quad (9)$$

as can be seen, e.g., from (53) and (19) of B53. The corresponding term of the inelastic contribution is

$$\tfrac{1}{4}Z\bar{\chi}_c^2 l(l+1)\ln(\chi_{\mathrm{in}}^{-2}) =\tfrac{1}{4}Z\bar{\chi}_c^2 l(l+1)[\ln(\chi_a^{-2})+\ln(\chi_a/\chi_{\mathrm{in}})^2]. \quad (10)$$

The combined dependence of the exponent of (1) on χ_a and χ_{in} is given by the sum of (9) and (10), namely

$$\tfrac{1}{4}Z(Z+1)\bar{\chi}_c^2 l(l+1) \times\{\ln(\chi_a^{-2})+(Z+1)^{-1}\ln(\chi_a/\chi_{\mathrm{in}})^2\}. \quad (11)$$

The first term in the braces, multiplied by the factor in front, coincides with the value derived by the Molière theory, as in B53, including the factor $Z(Z+1)$, which makes the estimated allowance for inelastic scattering. The second term in the braces represents the correction to the earlier estimate and may be looked upon as a change in the effective value of χ_a.

In the Molière theory, the cut-off angle χ_a is eventually incorporated in the parameter (19-B53), defined by

$$b=\ln(\chi_c/\chi_a)^2+1-2C. \quad (12)$$

The corrective term in (11) may be similarly incorporated by replacing b with

$$\bar{b}=b+(Z+1)^{-1}\ln(\chi_a/\chi_{\mathrm{in}})^2. \quad (13)$$

3. NUMERICAL ESTIMATE OF THE CORRECTION

According to (8) we write

$$\ln(\chi_a/\chi_{\mathrm{in}})^2 =\lim_{k=\infty}\left[2\int_0^k S(v)d\chi/\chi+1-2\ln k+2\ln\chi_a\right]. \quad (14)$$

For convenience of computation and in order to eliminate irrelevant physical quantities, we change the variable χ into

$$u=2\ln v\approx 2\ln\chi+2\ln(0.333Z^{-\frac{1}{3}}pa/\hbar). \quad (15)$$

[The exact form of this equation has $\ln(2(1-\cos\chi))$ in the place of $2\ln\chi$, but the small-angle approximation is already implied in (7) and (8).]

The cut-off angle χ_{in} defined by (8) is then replaced with

$$-u_{\mathrm{in}}=\lim_{U=\infty}\left[\int_{-\infty}^U S(\exp\tfrac{1}{2}u)\,du+1-U\right]. \quad (16)$$

The cut-off angle χ_a, whose value is given by (20) and (8) of B53, is replaced with

$$u_a=2\ln[Z^{\frac{1}{3}}(\hbar/pa)/0.885] +\ln(1.13+3.76zZe^2/\hbar v)+2\ln(0.333Z^{-\frac{1}{3}}pa/\hbar) =\ln[0.160Z^{-\frac{2}{3}}(1+3.33zZe^2/\hbar v)], \quad (17)$$

so that we write

$$\ln(\chi_a/\chi_{\mathrm{in}})^2=u_a-u_{\mathrm{in}}. \quad (18)$$

Equation (16) has been utilized for the computation of $-u_{\mathrm{in}}$ by graphical integration. Starting from the tabulated data on the function $S(v)$ from the Thomas-Fermi model,[8,9] one finds

$$(-u_{\mathrm{in}})_{\mathrm{T.F.}}=5.8 \quad (19)$$

for all Z. The value of $(-u_{\mathrm{in}})$ should not vary greatly from one material to another. For the H atom, $-u_{\mathrm{in}}$ can be calculated exactly and is 3.6. White[10] has analyzed available data on the function S and on the resulting value of $-u_{\mathrm{in}}$. For Li and O the values of $-u_{\mathrm{in}}$ from Hartree calculations are 4.6 and 5.0, respectively. The Thomas-Fermi value may be somewhat too large because of the excessive tail of S, which relates to

[7] Large angle corrections to (5) may be entered, if required, by treating the atomic electron as a free particle, in which case $S=1$ (see Secs. 4 and 5). Small-angle corrections would be required for values of χ no larger than the ratio I/T of the binding energy of atomic electrons to the kinetic energy of the incident particle. However such small deflections can be disregarded for our purpose, since the range $0\leqslant\chi\leqslant I/T$ does not contribute appreciably to the integral in (8) because the integrand $S(v)/\chi$ levels off at values of $\chi\gg I/T$.

[8] W. Heisenberg and L. Bewilogua, Physik. Z. **32**, 737, 740 (1931). The factor $Z^{-\frac{1}{3}}$ in the definition of v serves to minimize the variation of $S(v)$ from one material to another. The symbol v is frequently utilized as the variable of the scattering function and should not be easily confused with the velocity.

[9] See also J. A. Wheeler and W. E. Lamb, Jr., Phys. Rev. **55**, 858 (1939), and M. Pirenne (see reference 5).

[10] G. R. White, National Bureau of Standards Report No. 2763, 1953 (unpublished).

the incorrect feature of the T.F. model of having electrons with binding energies ranging all the way down to zero. The incoherent scattering function may also be calculated from the Wentzel atom model,[11] which relates it to the experimental value of the volume diamagnetic susceptibility $\chi_{\rm dia}$. This method yields

$$(-u_{\rm in})_W=\ln[Z^{\frac{1}{3}}(A/\rho)1.87\times10^6(-\chi_{\rm dia})], \quad (19')$$

where A and ρ are the atomic weight and the density of the material. This formula yields $-u_{\rm in}=6.3$ for Pb. Presumably $S(v)$ should approach the Wentzel value at low v and the Thomas-Fermi value at high v.[10,11]

4. LARGE ANGLE EFFECTS FOR INCIDENT ELECTRONS

Additional departures from the Molière theory results are caused by departures of the inelastic cross section from the Rutherford formula at large angles. The correct cross section for inelastic collisions of incident electrons with substantial deflection and energy loss is given by the Møller formula for collisions between free electrons. This formula departs from the Rutherford formula when the deflection χ attains either the order of 1 radian or the order of $(mc^2/E)^{\frac{1}{2}}$, E being the energy of the incident electron.

Deflections of this magnitude usually belong in the tail of the multiple-scattering distribution, that is, they happen once only, if at all, along the path length of interest. Under these conditions the correct angular distribution $f_{\rm corr}(t,\vartheta)$ may be estimated according to the formula

$$f_{\rm corr}(t,\vartheta)=f_{\rm Molière}(t,\vartheta)\{\sigma_{\rm exact}(\vartheta)/\sigma_{\rm Ruth.}(\vartheta)\}, \quad (20)$$

as suggested by Bethe (note on p. 1259 of B53).

Very high energies and rather long path lengths yield an increasing chance of repeated deflections large enough to involve appreciable departures from the Rutherford formula. This effect can be estimated by expanding the ratio $\sigma_{\rm Møller}/\sigma_{\rm Ruth.}$ into powers of $1-\cos\chi$ and incorporating one or two terms of the expansion in the calculation of (1). The resulting corrections are of the same order as the corrective term (54) of B53 and therefore should be considered only if one takes into account at the same time other corrections to the standard Molière theory.[1,2]

If the departures from the Rutherford formula are too large, the exponent of (1) cannot be represented adequately by the analytical expression suited for the Molière method of summation over l. A general method of numerical summation over l has been applied by Spencer and Blanchard[12] to multiple scattering in a gold foil. The results of this calculation lend support to the estimation of relativity corrections by means of (20).

[11] F. Lenz, Naturwiss. **39**, 265 (1952).

[12] See reference 6. See also L. V. Spencer, Phys. Rev. **90**, 146 (1953).

5. CALCULATION FOR INCIDENT HEAVY PARTICLES

The recoil imparted to atomic electrons by incident heavy particles cannot exceed a certain, comparatively low, ceiling. As the recoil momentum increases, the deflection χ experienced by the incident particle increases at first but then decreases back to zero as the ceiling is approached. The Rutherford cross section remains approximately correct if expressed as a function not of the deflection χ but of the recoil momentum or of the equivalent "recoil energy" Q, i.e., of the kinetic energy which would be absorbed by a free electron recoiling from rest.

The inelastic cross section (5) is anyhow expressed somewhat more accurately in the form

$$Nt\sigma_{\rm inel}(Q)dQ=Z\bar{\chi}_c^2S(v)(p^2/2m)dQ/Q^2, \quad (21)$$

with

$$v=0.333Z^{-\frac{2}{3}}(a/\hbar)(2mQ)^{\frac{1}{2}} \quad (22)$$

(m = electron mass), and with Q varying between the limits $Q_{\rm min}$ and $Q_{\rm max}$ of the stopping power theory.[13] The lower limit $Q_{\rm min}$ is effectively zero for our purpose (see note 7); the upper limit is given for heavy particles by (50.11) of B33, namely,

$$Q_{\rm max}=2mv^2/(1-v^2/c^2).^{14} \quad (23)$$

Equation (21) is formally equivalent to (5) provided one sets $2(1-\cos\chi)=2mQ/p^2$. Actually the relationship between χ and Q in a collision with energy loss ϵ is, to a good approximation,[15]

$$2(1-\cos\chi)=(2m/p^2)[Q-(\epsilon^2/2mv^2)(1-v^2/c^2)]. \quad (24)$$

The mean value of ϵ^2, averaged over all inelastic collisions with a fixed Q, can be derived by a sum rule and is $[Q^2+4Q\langle T\rangle/3]/S(v)$, where $\langle T\rangle$ indicates the mean kinetic energy of the atomic electrons. Therefore we write

$$\langle 2(1-\cos\chi)\rangle = (2mQ/p^2)[1-(Q+4\langle T\rangle/3)/Q_{\rm max}S(v)]. \quad (25)$$

The term with $\langle T\rangle/Q_{\rm max}$ yields a negligible contribution and will be disregarded in the following.

Equation (23) must further be modified by the insertion of a relativistic factor[16] on the right side,

[13] See, e.g., H. A. Bethe, *Handbuch der Physik* (Springer, Berlin, 1933), Vol. 24, Part 1, p. 491 ff., which will be referred to as B33; Eq. (21) is easily derived from (49.6) of B33.

[14] This formula holds only as long as the incident particle energy E divided by its rest energy Mc^2 remains much smaller than $M/2m$.

[15] This formula constitutes the zero-order term of an expansion in powers of ϵ/pv, a parameter which is always very small for incident heavy particles. Notice how the right side of (24) vanishes for $Q=Q_{\rm min}$ and also, for heavy particles only, when $Q=\epsilon=Q_{\rm max}$.

[16] The relativistic treatment of inelastic collisions given in B33 (esp. p. 506) and in the original literature, is not as exhaustive as one might wish. The main question concerns the evaluation of the relativistic form factor (50.2) of B33. It is stated that the relativistic and non-relativistic form factors differ appreciably only for values of Q much lower or much larger than the binding energy of the atomic electrons. The reason is that the relativistic effect depends on the speed of atomic electrons which is itself

according to (55.7) of B33, namely,

$$1-(Q/2mc^2)(1-v^2/c^2)=1-(Q/Q_{\max})(v^2/c^2). \quad (26)$$

We wish now to calculate, for incident heavy particles, the full contribution of inelastic collisions to the exponent of (1). The integral over χ has to be transformed into an integral over Q. The factor $1-P_l(\chi)$ in (1) can be represented as a polynomial in $1-\cos\chi$, of which only the first degree term is significant, since $1-\cos\chi$ never exceeds $\frac{1}{4}(m/M)^2$, where M is the mass of the incident particle,

$$1-P_l(\chi)=\tfrac{1}{2}l(l+1)(1-\cos\chi), \quad \text{for} \quad l\ll M/m.^{17} \quad (27)$$

The value of $1-\cos\chi$ in terms of Q is given by (25). Combining (21), (22), (25), (26), and (27) we find that the inelastic component to the exponent of (1) is:

$$\tfrac{1}{4}Z\bar{\chi}_c^2 l(l+1)D, \quad (28)$$

where

$$D=\int_{Q_{\min}}^{Q_{\max}} dQQ^{-1}[S(v)-Q/Q_{\max}] \times[1-(Q/Q_{\max})(v^2/c^2)]$$
$$=\left\{\int_{u_m}^{u_M} S(\exp\tfrac{1}{2}u)du-\int_{Q_{\min}}^{Q_{\max}} dQS(v)Q_{\max}^{-1}(v^2/c^2) -(1-Q_{\min}/Q_{\max})+\tfrac{1}{2}(1-Q_{\min}^2/Q_{\max}^2)(v^2/c^2)\right\}, \quad (29)$$

and

$$u_M=\ln[(0.333)^2Z^{-4/3}2mQ_{\max}a^2/\hbar^2] =\ln[8340Z^{-4/3}(c^2/v^2-1)^{-1}], \quad (30)$$

$$u_m=\ln[(0.333)^2Z^{-4/3}2mQ_{\min}a^2/\hbar^2]. \quad (31)$$

usually (but not for internal electrons and high Z) non-relativistic, except when Q itself approaches mc^2. For Q near $Q_{\min}$ the correction becomes appreciable because the nonrelativistic form factor tends to vanish. This effect is unimportant for us, because low Q values contribute negligibly to multiple scattering. The high Q correction is represented for heavy particles by the factor (25), for incident electrons by the replacement of the Rutherford with the Møller formula.

[17] If (27) holds for all important values of l, the inelastic component to the exponent of (1) is proportional to $l(l+1)$, as calculated below, and its Legendre transform is Gaussian.

The first integral in the braces may be taken as $u_M-u_{\text{in}}-1$, according to (16), since u_m is effectively $-\infty$. In the second integral we can set $S(v)=1$, since the range of low Q contributes little. Finally $Q_{\min}/Q_{\max}$ can be disregarded when compared with 1. Therefore the value of (28) is

$$D=\ln[1130Z^{-4/3}(c^2/v^2-1)^{-1}]-u_{\text{in}}-\tfrac{1}{2}v^2/c^2. \quad (32)$$

The contribution of elastic collisions to the exponent of (1) may be written, according to (53) of B53, as $\frac{1}{4}Z^2\bar{\chi}_c^2 l(l+1)[b-\ln\frac{1}{4}y^2]$. Therefore the contribution (28) may be incorporated into the Molière theory according to the following prescription:

(a) take χ_c^2 as $Z^2\bar{\chi}_c^2$ rather than $Z(Z+1)\bar{\chi}_c^2$,

(b) add to b the quantity $Z^{-1}D$, where D is given by (32).

6. LIMITATIONS OF THE THEORY

The main limitation of the present theory probably lies in the acceptance of the Bethe theory of inelastic collisions, which assumes the incident particle to be much faster than the atomic electrons. This assumption is often not satisfied, e.g., for heavy particles of moderate energy or for high-Z atoms. Improvements over this initial assumption are often introduced in the theory of stopping power but have not been attempted in the present theory. However, inelastic collisions have substantial effect only in low-Z materials, where the assumption is best fulfilled. The simplifications made in the analytical development are believed accurate to within the limits of the Bethe theory of collisions.

Finally, both the present theory and the Molière theory assume that the characteristics of atomic structure affect $\sigma(\chi)$ only at such low values of χ that they do not influence the value of $\int_0^\pi\sigma(\chi)(1-\cos\chi)^n \sin\chi d\chi$ for $n\geqslant 2$.[18] This assumption may be not quite adequate for high-Z atoms.

[18] A calculation of the effect of atomic structure upon the integral for $n=2$ would correspond to the correction to the Landau theory of energy straggling introduced by O. Blunck and S. Leisegang, Z. Physik 128, 500 (1950).