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STOPPING OF SLOW H-, He-, Li- AND Be-LIKE PROJECTILES IN ELECTRON GAS*

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Results of calculations of the electronic stopping power and the energy loss straggling for low velocity H-, He-, Li- and Be-like projectiles in the degenerate electron gas are reported. The Hartree–Fock–Slater description of the projectile and the dielectric function method were used. The size parameter $Z_{\rm min}$ of the charge distributions calculated from a variational principle depends on the characteristics of the medium. The stopping and straggling effective charges $Z_{\rm ef}$ of a projectile were analysed. They were found to differ with each other and to depend on the one-electron radius r_s, on the projectile atomic number Z_i and on the number of electrons N_i carried by the projectile.

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1. Introduction

After crossing the surface of a solid a slow atomic nucleus captures electrons forming intermediate electronic configurations up to being almost completely neutralised as it stops. This configuration strongly modifies the electronic stopping power and the energy loss straggling for the ion beam, which are important in analysis of distribution and lattice localisation of implanted atoms or in analysis of surface structure. The most important works in this field [1–5] were related to analysis of the stopping and straggling of an atomic nucleus as a projectile and neglecting thus an effect of its electronic configuration. A common feature of these theories is proportionality of the stopping power to velocity v and the energy loss straggling to v^2. The target and the projectile dependencies contained in the proportionality factor are model-dependent and they are different. The target, which consists of the free electron gas (at $T = 0$ K), is characterised by the one-electron radius r_s ($n = 3/4\pi r_s^3 a_0^3$ is the electron gas density). The projectile consists of an

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atomic nucleus of atomic number Z_i, moving slowly with velocity v and carrying N_i electrons.

In this paper m, e, a_0, and v_0 are the electron rest mass, the elementary charge, the Bohr radius, and the Bohr velocity, respectively. Atomic units are used throughout.

2. Calculation procedure

The probability for transfer of the energy ω and the momentum k to a degenerate free electron gas from a projectile is described within the random phase approximation (RPA) by the equilibrium dielectric function $\epsilon(k,\omega)$. Commonly the dimensionless parameters $z = k/2k_{\mathrm{F}}$, $u = \omega/kv_{\mathrm{F}}$ and $\chi^2 = r_{\mathrm{s}}/\pi\alpha$ are used, where $k_{\mathrm{F}} = \alpha/a_0 r_{\mathrm{s}}$ is the modulus of the Fermi wave vector and $\alpha = (9\pi/4)^{1/3}$. The electronic stopping cross-section S and the straggling parameter Ω^2 (per free electron) for a projectile of velocity v are given by [1, 2]:

$$S = \frac{1}{n}\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{4\pi e^4}{mv^2}Z_i^2 L_1, \qquad \frac{1}{n}\frac{\Omega^2}{x} = \frac{4\pi e^4}{mv^2}Z_i^2 L_2, \tag{1}$$

where

$$L_m = (4E_{\mathrm{F}})^{m-1}\frac{6}{\pi\chi^2}\int_0^{v/v_{\mathrm{F}}} \mathrm{d}u u^m \int_0^{\infty} \mathrm{d}z z^m Z^2(z) \Im\left[\frac{1}{\epsilon(u,z)} - 1\right], \tag{2}$$

where the dielectric function reads $\epsilon(u,z) = 1 + (\chi^2/z^2)[f_1(u,z) + \mathrm{i}f_2(u,z)]$, $E_{\mathrm{F}} = \alpha^2/2r_{\mathrm{s}}^2$ is the Fermi energy, and the factor $4\pi e^4/mv^2 = 4\pi e^2 a_0 (v_0/v)^2$. The form factor $Z^2(z)$ is the Fourier transform of the spatial electron distribution on the projectile [6–8] being a sum of the screening component Z_{s}^2 and the anti-screening component Z_{a}^2,

$$Z^2(z) = Z_{\mathrm{s}}^2(z) + Z_{\mathrm{a}}^2(z) = [1 - \rho(z)N_i/Z_i]^2 + \{1 - [\rho(z)]^2\}N_i/Z_i^2, \tag{3}$$

where $\rho(z)$ is the one-electron form factor.

Explicitly Eq. (2) takes the form

$$L_m = -(4E_{\mathrm{F}})^{m-1}\frac{6}{\pi}\int_0^{v/v_{\mathrm{F}}} \mathrm{d}u u^m \int_0^{\infty} \mathrm{d}z \frac{z^{m+2}Z^2(z)f_2(u,z)}{[z^2 + \chi^2 f_1(u,z)]^2 + [\chi^2 f_2(u,z)]^2}. \tag{4}$$

The conduction electrons of a solid screen the quasi-static electric potential of a slow projectile due to dielectric response. Provided the speed of the atom is lower than the Fermi velocity v_{F}, this screening can be approximately described in terms of the Coulomb potential between charges with the screening function $\exp(-rk_{\mathrm{TF}})$, where the Thomas–Fermi wave number k_{TF} is related to the Fermi wave number as $k_{\mathrm{TF}}^2 = 4k_{\mathrm{F}}/\pi a_0$. In this approximation we neglected to account for the full Lindhard dielectric function. More precisely, instead of the exponential decay the screening function displays rather the Freedel oscillations $V \propto \cos(rk_{\mathrm{TF}})/r^3$ caused by sharpness of the Fermi surface at $T = 0$ K.

The size parameter of bound electrons cloud can be determined either statistically or quantum mechanically. We want to determine stopping and straggling characteristics of the electron gas for an extended charge projectile by means of a size parameter of the charge distribution. This parameter is modified when the projectile enters a solid. When we deal with slow heavy projectiles carrying many electrons, then the statistical description and the density functional method are justified. When we consider projectiles with a small number of electrons the Hartree–Fock–Slater (HFS) description must be used. The intermediate region cannot be treated analytically.

We determine the volume parameter λ from the condition of minimum for the expectation value $\overline{H}$ of the total self-consistent Hamiltonian given (in hartree units) by

$$H = -\frac{1}{2}\sum_j \Delta_j - Z_i \sum_j \frac{\exp(-r_j k_{\mathrm{TF}})}{r_j} + \frac{1}{2}\sum_{j\neq k} \frac{\exp(-k_{\mathrm{TF}}|r_j - r_k|)}{|r_j - r_k|}, \tag{5}$$

with the orthonormal, one-electron trial eigenfunctions forming the HFS determinant ($\lambda = a_0/Z$ or Z alone are variational parameters)

$$u_{1s}(r) = \pi^{-1/2}(\lambda)^{-3/2}\exp(-r/\lambda),$$

$$u_{2s}(r) = \pi^{-1/2}(2\lambda)^{-3/2}(1 - r/2\lambda)\exp(-r/2\lambda). \tag{6}$$

The expectation values for the total Hamiltonian describing different $1s2s$ configurations can be calculated as

$$\overline{H}(\mathrm{H} \equiv 1s^1) = E_{1s},$$

$$\overline{H}(\mathrm{He} \equiv 1s^2) = 2E_{1s} + V_{1s1s},$$

$$\overline{H}(\mathrm{Li} \equiv 1s^2 2s^1) = 2E_{1s} + E_{2s} + V_{1s1s} + 2V_{1s2s} - A_{1s2s},$$

$$\overline{H}(\mathrm{Be} \equiv 1s^2 2s^2) = 2E_{1s} + 2E_{2s} + V_{1s1s} + V_{2s2s} + 4V_{1s2s} - 2A_{1s2s}, \tag{7}$$

where the eigenenergies (E), the Coulomb (V), and the exchange (A) integrals are given in Appendix.

The Fourier transform of the spatial electron distribution on the projectile carrying N_{1s} electrons in the $1s$ state and N_{2s} electrons in the $2s$ state ($N_i = N_{1s} + N_{2s}$) from Eq. (6) reads

$$N_i\rho(z) = N_{1s}\rho_{1s}(2\phi) + N_{2s}\rho_{2s}(2\phi)$$

$$= N_{1s}\frac{1}{(1+\phi^2)^2} + N_{2s}\frac{1 - 3(2\phi)^2 + 2(2\phi)^4}{[1+(2\phi)^2]^2}, \tag{8}$$

where $\phi = k_{\mathrm{F}}\lambda z$.

3. Results and discussion

We carried out calculations for extended charge projectiles moving slowly in the uniform electron gas. We get analytical results for the stopping power and for the energy loss straggling for the gas described by Lindhard's dielectric function $\epsilon(u,z) = 1 + (\chi^2/z^2)[f_1(u,z) + \mathrm{i}f_2(u,z)]$ [1, 2]. The L_m functions of Eq. (4) are expressed as

$$L_m = (3E_{\mathrm{F}})^{m-1}\left(\frac{v}{v_{\mathrm{F}}}\right)^{m+2} C_m, \quad C_m = \int_0^1 \mathrm{d}z\, z^{m+2}\frac{Z^2(z)}{[z^2 + \chi^2 f_1(0,z)]^2}. \tag{9}$$

The variable $u = m\omega/kk_\mathrm{F} = \hbar\omega/zE_\mathrm{F}$ measures the energy $\hbar\omega$ (in units of the Fermi energy E_F) transferred from the projectile to the medium. For slow projectiles the energy transfer is very low, i.e. $u \ll 1$, therefore the approximation leading from Eq. (4) to Eq. (9) is justified. In this case the approximation $f_1(0,z) = 1 - z^2/3$ can be used, therefore the denominator in Eq. (9) reads $[z^2 + \chi^2(1-z^2/3)]^2 = (\chi^2/\chi'^2)^2(z^2+\chi'^2)^2$, where $\chi'^2 = \chi^2/(1-\chi^2/3)$. For real metals $1.5 < r_\mathrm{s} < 5.8$, therefore $0.50 < \chi < 0.98$ and $0.52 < \chi' < 1.19$.

From Eq. (1), in atomic units (hartree/a_0 and hartree$^2/a_0$), we get

$$\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{4}{3\pi}\frac{v}{v_0}Z_i^2C_1, \qquad \frac{\Omega^2}{x} = \frac{9}{r_\mathrm{s}^3}\left(\frac{v}{v_0}\right)^2 Z_i^2C_2. \tag{10}$$

For heavier ions carrying many electrons we get analytical formulas for C's cited in the previous paper [9].

In the case of projectiles carrying a small number of electrons in the $1s$ and $2s$ states and described by the form factor from Eq. (3) we get the functions C_1 and C_2 in closed analytical forms. They depend on $(Z_i, r_\mathrm{s}, N_{1s}, N_{2s})$ parameters. Due to their complicated forms they will not be presented here, but can be obtained from the author on request. The analytical result allows for power expansion, contrary to the direct numerical integration in Eq. (9). L_1 and C_m are dimensionless and L_2 is expressed in atomic hartree units.

This formulas are directly reduced to the case of an atomic nucleus by setting $N_i = 0$. From Eq. (9) we get

$$C_1 = 0.5\left[-\frac{1}{1+\chi'^2} + \ln\left(1+\frac{1}{\chi'^2}\right)\right],$$

$$C_2 = 1 + 0.5\left(\frac{\chi'^2}{1+\chi'^2} - 3\chi'\arctan\frac{1}{\chi'}\right). \tag{11}$$

When a projectile with few electrons moves in the vacuum then $\gamma = 0$, and then the $\overline{H}$'s of Eq. (7) reach minima (calculated from the requirement $\partial\overline{H}/\partial Z = 0$) at Z_min equal to $Z_\mathrm{H} = Z_i$, $Z_\mathrm{He} = Z_i - 0.3125$, $Z_\mathrm{Li} = Z_i - 0.45458$ and $Z_\mathrm{Be} = Z_i - 0.6284$, for hydrogen-, helium-, lithium- and berilium-like electronic configurations, respectively. The corresponding energy minima are: $\overline{H}_\mathrm{He} = -Z_\mathrm{He}^2$, $\overline{H}_\mathrm{Li} = -(9/8)Z_\mathrm{Li}^2$, $\overline{H}_\mathrm{Be} = -(5/4)Z_\mathrm{Be}^2$ in hartree units. When the projectile moves slowly in a solid, keeping all the time a stable electronic configuration, these parameters are modified due to interaction with electron gas. For each electronic configuration the screening parameter λ (Z_min) was calculated by taking numerically minimum of the appropriate $\overline{H}$ from Eq. (7), therefore λ depends on Z_i, N_i, and additionally on r_s. Subsequently λ was used in Eqs. (8, 3).

This solid state effect on screening was shown in Fig. 1. We plot the difference $Z_i - Z_\mathrm{min}$ for Be-like projectiles, as a function of Z_i and r_s. It is obvious that all such Z_min functions tend to the above limits in the dilute electron gas, as r_s is large. For a dense electron gas (small r_s) the functions are larger than the limits, which means stronger screening of the projectile nucleus interaction by the medium. This screening is more important at low Z_i.

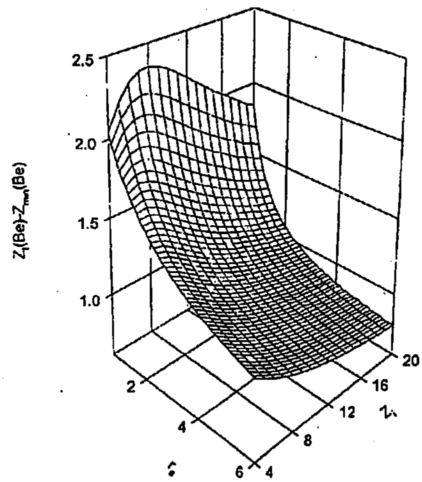

Fig. 1. The parameter $Z_{\rm min}$ calculated for Be-like projectiles of atomic number Z_i. The atomic and the screening effects are included.

The common feature of the present and other results is that the stopping power S is proportional to v and the energy loss straggling Ω^2 to v^2 at low ion velocity v. The differences are model-dependent and are related to the coefficient of proportionality $C(Z_i, r_{\rm s}, N_{1s}, N_{2s})$ which incorporates both the target parameter $r_{\rm s}$ and the projectile parameters Z_i, N_{1s}, and N_{2s}. They cannot be further simplified or separated even after power expansion.

In order to perform calculations we assume a stable in time, frozen charge distribution on the projectile. Within this model [6, 7, 9] the projectile charge in the Fourier space which contributes to Eq. (9) is a sum of the screening component $[1 - \rho(z)N_i/Z_i]^2$ and the anti-screening component $\{1 - [\rho(z)]^2\}N_i/Z_i^2$. As long as we deal with slow, heavy projectiles, considering only the screening component is justified. For light and neutral projectiles the anti-screening must be taken into account, since it enhances the stopping and straggling by about 10%. From Eq. (3) we find that in the low momentum transfer limit $Z^2(0) = [1 - N_i/Z_i]^2$ we get reduction of soft, distant collisions contribution to the loss process. The large momentum transfer limit $Z^2(\infty) = 1 + N_i/Z_i^2$ gives enhancement of the contribution from hard, close collisions due to excitations of the electron gas by projectile electrons.

In order to analyse results we should realise that dependence of C's on Z_i means that the proportionality of the energy loss and the straggling to Z_i^2, correct for a point charge, is broken in a case of an extended charge, and the projectile excites the medium as a stable charge configuration. The behaviour of C's with $r_{\rm s}$ can be understood by noting that the energy absorbed by the electron gas on collective excitations drops as $r_{\rm s}^{-3/2}$ and the number of electrons subjected to the single particles excitations are related to the density of states below the Fermi level $E_{\rm F}$.

From the previous paper [10] (when statistical description of the projectile electrons is applied), if we expand C_1 and C_2 in a power series we find that for a dense medium and for a heavy projectile $C_1 \propto r_s^4 Z_i^{-4/3}$ and $C_2 \propto r_s^2 Z_i^{-2/3}$. From Eq. (10) we get $\mathrm{d}E/\mathrm{d}x \propto Z_i^{2/3}$ and $\Omega^2/x \propto Z_i^{4/3}$, respectively.

For the energy loss analysis the concept of effective charge is applied [6, 7, 9]. It relates the stopping and straggling produced by a given projectile to the same characteristics produced by the projectile atomic nucleus. We define the effective charge for the stopping Z_{ef1} and for straggling Z_{ef2} separately as

$$Z_{\mathrm{ef}m} = \sqrt{C_m(Z_i, r_\mathrm{s}, N_{1s}, N_{2s})/C_m(Z_i, r_\mathrm{s}, 0, 0)}. \tag{12}$$

For a point charge $Z_{\mathrm{ef}m} = 1$. An independence of $Z_{\mathrm{ef}m}$ on Z_i means that the Bethe Z_i^2 scaling is only accidentally valid for both stopping and straggling. This scaling is related to the same contribution of close and distant collisions in the process of energy transfer to the electron gas. In the static case the result $Z_{\mathrm{ef}} < 1$ means that projectile electrons screen the Coulomb potential of the projectile nucleus. As an example we have shown in Fig. 2 the stopping power effective charge Z_{ef1} for Li-like projectiles. In the dilute electron gas ($r_\mathrm{s} = 6$) and for low projectile atomic number Z_i the effective charge is much smaller than unity, $Z_{\mathrm{ef1}} \ll 1$. For large Z_i it tends slowly to unity.

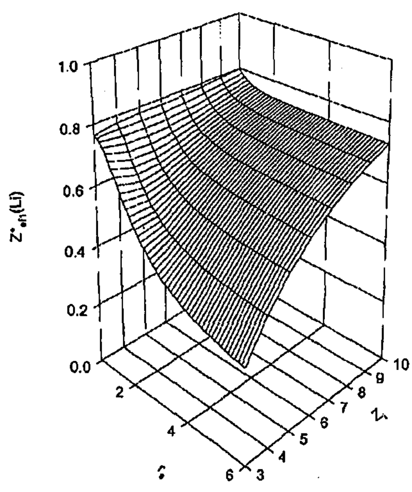

Fig. 2. The stopping effective charge for Li-like projectiles.

It is of interest to see how large are the atomic and the electron gas screening contributions calculated for Z_{min}, when compared to the $Z_{\mathrm{min}} = Z_i$ case. The difference between the stopping power effective charges Z_{ef1} are plotted in Fig. 3 as a function of r_s and Z_i for Be-like projectiles. It reaches maximum at $r_\mathrm{s} = 0.7$ for small Z_i and rapidly decreases to zero as Z_i increases. The energy straggling effective charge Z_{ef2} displays the similar behaviour.

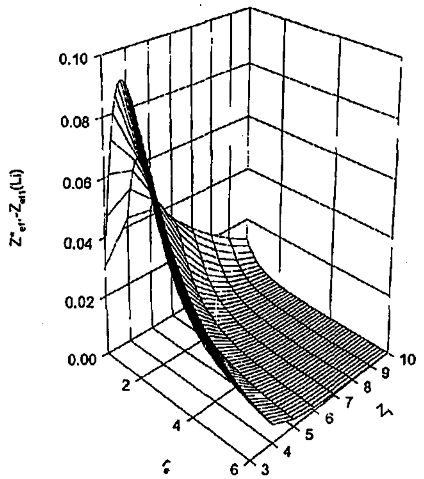

Fig. 3. The effect of switching on the atomic and the screening contributions to the calculation of the stopping effective charge for Li-like projectiles. Z_{ef1} is calculated by taking $Z_{min} = Z_i$.

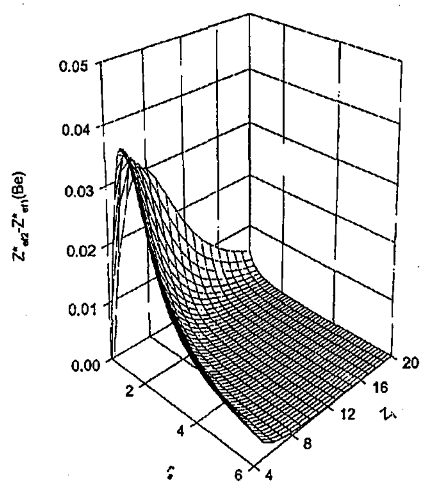

Fig. 4. Difference between the straggling effective charge Z_{ef2} and the stopping effective charge Z_{ef1} for Be-like projectiles.

In Fig. 4 the differences between the effective charges for straggling and for stopping $Z_{ef2} - Z_{ef1}$ is shown for Be-like projectiles as a function of r_s versus Z_i. The atomic and the solid state effects were included here through Z_{min} calculated by taking minimum of $\overline{H}(\text{Be} = 1s^2 2s^2)$ in Eq. (7). The differences between both effective charges are r_s dependent (they amount to 3.5%) for small Z_i and tend to zero as Z_i increases. This interesting feature is caused by a structure of the integrals in Eq. (9).

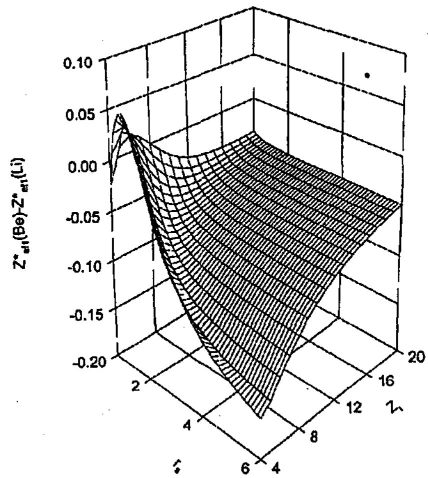

Fig. 5. The influence of one additional $2s$ electron on the stopping power effective charge between Li-like and Be-like projectiles.

Another interesting question is how the effective charge will change, when we add (or remove) one electron to (from) the projectile. In Fig. 5 we have shown the difference between the stopping effective charge $Z_{\rm ef1}$ for a Be-like projectile of the net charge Z_i-4 and the stopping effective charge $Z_{\rm ef1}$ for a Li-like projectile of the net charge Z_i-3. Nearly for all r_s and Z_i, $Z_{\rm ef1}(\rm Be) < Z_{\rm ef1}(\rm Li)$. Asymptotically, for large Z_i, adding one electron to the projectile causes negligible decrease in the effective charge. For a dilute electron gas and for small Z_i this difference reaches 0.2. For a dense ($r_s = 0.7$) electron gas the situation is opposite: $Z_{\rm ef1}(\rm Be) > Z_{\rm ef1}(\rm Li)$ which means that a Be-like projectile transfers the energy to the medium more effectively than a Li-like projectile.

4. Conclusions

Result of the calculation for the electronic stopping power and the energy loss straggling of free electron gas for low velocity H-, He-, Li- and Be-like projectile was presented. The Hartree–Fock–Slater description of the projectile in a solid was used. The size parameter λ (or Z) was determined from a variational principle and shown to depend on r_s, Z_i, N_{1s}, and N_{2s}. The anti-screening correction was included and found to be important for small Z_i. The dependence of the effective ion charges on the target electron gas density r_s and on the projectile atomic number Z_i and the number of electrons on the projectile was discussed.

Appendix

The eigenenergies (E), the Coulomb (V), and the exchange (A) integrals were calculated as ($\gamma = k_{\rm TF}\lambda$ and $\gamma' = 2\gamma/3$)

$$E_{1s} = \frac{e^2}{a_0}\left[\frac{Z^2}{2} - \frac{Z_i Z}{(1+\gamma/2)^2}\right], \tag{13}$$

$$E_{2s} = \frac{e^2}{a_0}\left[\frac{Z^2}{8} - \frac{Z_i Z}{4(1+\gamma)^2}\left(2 - \frac{4}{(1+\gamma)} + \frac{3}{(1+\gamma)^4}\right)\right], \tag{14}$$

$$V_{1s1s} = \frac{e^2}{a_0} Z \frac{5+\gamma+\gamma^2/4}{8(1+\gamma/2)^4}, \tag{15}$$

$$V_{2s2s} = \frac{e^2}{a_0} Z \frac{77 + 104\gamma + 227\gamma^2 + 144\gamma^3 + 123\gamma^4 + 40\gamma^5 + 5\gamma^6}{512(1+\gamma)^4}, \tag{16}$$

$$V_{1s2s} = \frac{e^2}{a_0} Z \frac{4}{81} \frac{17 + 4\gamma + 21\gamma^2 + 8\gamma^3 + \gamma^4}{(1+\gamma)^4 (2+\gamma)^2}, \tag{17}$$

$$A_{1s2s} = \frac{e^2}{a_0} Z \frac{16}{729} \frac{3 - 25\gamma'^2 + 150\gamma'^4 - 256\gamma'^5 + 150\gamma'^6 - 25\gamma'^8 + 3\gamma'^{10}}{3(1-\gamma'^2)^6}. \tag{18}$$

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