Dynamic shadow effect in energy losses experienced by heavy charged particles

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A nonrelativistic quantum-mechanical Glauber–Franco approximation for the inelastic scattering amplitude is used in an analysis of the energy losses due to the excitation and ionization of atoms in an amorphous target by heavy particles carrying a unit charge. The results of calculations of the energy losses of protons in H and He targets are in good agreement with the experimental data. The agreement is due to an allowance for the nuclear dynamic shadow effect and for the redistribution of energy between electrons of the target atoms. Expressions are obtained for calculation of the energy losses allowing for the individual characteristics of occupancy of the electron shells of the target atoms.

1. INTRODUCTION

Extensive use of ion beams for the analysis of surface layers of materials and studies of the distributions of implanted ions depend on detailed information on the energy losses in a wide range of energies, particle charges $Z_1 e$, and atomic numbers of the target material Z_2. Due to certain experimental limitations, the data on the energy losses can be obtained only for limited ion–target combinations. On the other hand, there is no general theory which would make it possible to calculate the energy losses experienced by ions of all velocities and for all combinations of Z_1 and Z_2. Therefore, a scaling relationship is used in systematic presentation of the data, because this makes it possible to represent the loss function as a product of two functions, one of which depends solely on the ion charge and velocity and the other depends on the ion velocity and on parameters representing the target material. It follows from the results of Refs. 1–4 that this relationship is valid to within $\sim 10\%$ and that its application makes it possible to find the energy losses for different values of Z_1 and Z_2, and for different energies utilizing the results of direct measurements for individual elements. The experimental data used most frequently for this purpose are those on the energy losses of protons ($Z_1 = 1$) experienced by various substances, which are known to a high degree of accuracy and for a wide range of velocities. We therefore consider the energy losses of heavy particles with a unit (proton) charge.

In general, the energy lost by a charged particle is governed by a variety of processes, so that a theoretical description becomes very complicated. However, the contributions of these processes to the total losses depend strongly on the proton velocity. At very low velocities ($E \lesssim 100$ eV) the losses are primarily through elastic scattering on the target atoms. The monograph of Gott[5] gives the expressions for the calculation of the energy losses derived using the Thomas–Fermi–Firsov potential[6] and other approximations for the potential energy of the interaction, and it is shown there that the contribution of elastic collisions to the total losses decreases rapidly as the proton velocity increases. At moderate velocities, which are still less than the average velocity of atomic electrons, the energy losses experienced by protons are governed by the electron exchange process. As shown in Refs. 7–10, the energy losses are proportional to the velocity of a heavy particle. This is supported by the experimental data, although there are some deviations from this law (see, for example, Ref. 11).

If the proton velocity is much higher than the average velocity of atomic electrons ($v_e = e^2/\hbar$), the energy losses are determined by the processes of excitation and ionization of the target atoms. A detailed theoretical calculation of the losses in this range, based on the use of the first Born approximation for the inelastic scattering amplitude, was given in the monograph of Mott and Massey.[12] The use of the Born approximation implies that the amplitude of a wave scattered by atomic electrons is small compared with the amplitude of the incident wave. The condition for the validity of the Born approximation ($Z_1 e^2/\hbar v \ll 1$, where v is the proton velocity) allows us to ignore charge-exchange processes. If the proton velocity satisfies this condition, the expression for a calculation of the energy losses is

$$\frac{dE}{dx} = \frac{4\pi N_0 e^4}{mv^2} Z_2 \ln\left(\frac{2mv^2}{I_z}\right), \tag{1}$$

where m is the mass of an electron; N_0 is the number of atoms per unit volume; I_z is the average ionization energy of an atom. An estimate of I_z obtained using the Thomas–Fermi model gives the dependence $I_z \approx I_0 Z_2$, where I_0 is a constant whose value can be determined experimentally.[12] The model of local oscillators was used in Ref. 13 to calculate the values of I_0 for all the elements. However, one should mention serious discrepancies between the calculated and experimental values of this quantity.[14]

Equation (1) describes well the experimental data for fast particles. We can extend the range of validity of this expression by calculating the relativistic corrections as well as the corrections allowing for the shell structure of the atoms. The effect of an incident particle perturbing electrons was also allowed for in Ref. 15, which made it possible to derive a correction to Eq. (1) proportional to Z_1^3. However, at a proton velocity comparable with the average velocity of electrons of the target atoms the Bethe–Bloch expression (1) overestimates the losses (compared with the experimental values) even when corrections are made. It is then necessary to use empirical expressions to calculate the losses (see, for example, Ref. 6) or fitting parameters[9,16,17] in order to ensure agreement with the experimental results.

The use of empirical formulas and fitting parameters makes it difficult to understand the physical nature of the

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energy loss processes. This is particularly true in the case of the Z_2 oscillations. It is known that when the velocity of a heavy particle is comparable with the average velocity of atomic electrons, the dependence of the losses on Z_1 and Z_2 become nonmonotonic,[18,19] and the amplitude of the loss oscillations increases as the particle velocity is reduced. The model of local oscillators[20] is used in Refs. 21 and 22 to calculate the energy losses employing the atomic wave functions. This gave a nonmonotonic dependence on the parameters Z_1 and Z_2. However, the physical origin of this dependence remains unclear, since empirical parameters were used in the calculations.

The expression (1) for the energy losses was derived using the first Born approximation for the scattering amplitude. Note that the Glauber approximation[23] has been used successfully in the scattering theory in order to calculate the elastic and inelastic cross sections of collisions of electrons with atoms in the target.[24,25] The results of applying this approximation to slow electrons are in better agreement with the experimental data than those obtained employing the Born approximation.[26-27] An important feature of this approximation is that it allows for the potential interaction between a passing particle and a nucleus in all orders of perturbation theory and also that it satisfies the optical theorem. In calculating the cross sections by this approach we have to determine complex integrals,[28] but since the energy losses contain integrated information on the scattering process, the expressions should be relatively simple. Later we show that if we go beyond the Born approximation, we find that we can describe correctly the dependence of the energy losses on the proton velocity without introducing any fitting parameters and we can also allow consistently for the effects associated with the distribution of electrons in the target atoms, as well as provide physical interpretation of the results obtained. In the subsequent calculations we shall ignore both the electron exchange processes and the radiation-induced deceleration as well as the relativistic corrections, i.e., we shall consider only the losses due to the excitation and ionization of the target atoms. This limits the range of the relevant velocities of heavy particles to

$$v_e < v \ll c/Z_2^{1/2}, \tag{2}$$

where c is the velocity of light.

2. RELATIONSHIP DESCRIBING EFFECTIVE DECELERATION

To calculate the energy losses experienced by a heavy particle with a unit charge moving at a velocity v we shall use a relationship for the effective deceleration, which is governed by the sum of the products of the cross sections representing the transition of an atom from its ground state to any excited state and the corresponding energy of the transition.[29] If we assume that the inelastic scattering by individual atoms of the target material represents statistically independent events (which is not true of ordered media and structures), we obtain

$$\frac{dE}{dx} = N_0 \frac{2\pi}{kk_0} \sum_{\alpha} (E_\alpha - E_0) \int_{q_\alpha}^{q_m} q\, dq\, |f_{0\alpha}(\mathbf{q})|^2. \tag{3}$$

Equation (3) describes the effective deceleration in collisions in which the transferred momentum lies within the range from q_α to q_m. In Eq. (3) the quantities E_0 and E_α are the energies of the ground and excited states of an atom, and $f_{0\alpha}$ is the amplitude of the inelastic scattering process. The summation should be carried out using a set of quantum numbers of states in discrete $[\alpha = (n,l,m_l,s,m_s)]$ and continuous $[\alpha = (\mathbf{p},\mathbf{p}')]$ spectra; k_0 and k are the values of the wave vector of the heavy particle before and after the scattering; $q_m = 2mv/\hbar$ is the maximum possible momentum transferred in the course of a collision; $q_\alpha = (E_\alpha - E_0)/\hbar v$ is the minimum possible transferred momentum. It should be pointed out that in general both q_m and q_α depend on E_α.

We divide the integration range in Eq. (3) in terms of the variable q into two parts: $q_\alpha \leqslant q \leqslant q_0$ and $q_0 \leqslant q \leqslant q_m$, where $q_0 = I_0/\hbar v$ and I_0 is the ionization energy of an atom. We then have

$$\frac{dE}{dx} = \left(\frac{dE}{dx}\right)_\alpha + \left(\frac{dE}{dx}\right)_I, \tag{4}$$

where

$$\left(\frac{dE}{dx}\right)_\alpha = N_0 \frac{2\pi}{kk_0} \sum_{\alpha} (E_\alpha - E_0) \int_{q_\alpha}^{q_0} q\, dq\, |f_{0\alpha}(\mathbf{q})|^2, \tag{5}$$

$$\left(\frac{dE}{dx}\right)_I = N_0 \frac{2\pi}{kk_0} \sum_{\beta} (E_\beta - E_0) \int_{q_0}^{q_m} q\, dq\, |f_{0\beta}(\mathbf{q})|^2. \tag{6}$$

Equation (5) governs the energy losses due to the processes of excitation of an atom, whereas Eq. (6) represents those due to the ionization processes. Therefore, integration with respect to the momentum of an escaping electron is understood in Eq. (6), whereas summation is carried out over the quantum numbers. As pointed out in the Introduction, the inelastic scattering amplitude will be described by the Glauber–Franco approximation.[23,24] In this approximation we have

$$f_{\alpha 0}(\mathbf{q}) = \int d\tau\, \psi_\alpha^*(\mathbf{r})\, G(\mathbf{r},\mathbf{q})\, \psi_0(\mathbf{r}), \tag{7}$$

where

$$G(\mathbf{r},\mathbf{q}) = \frac{ik}{2\pi} \int d\mathbf{b} \exp(i\mathbf{qb}) [1 - \Gamma(\mathbf{b},\mathbf{r})], \tag{8}$$

and the phase function Γ is of the form

$$\Gamma(\mathbf{b},\mathbf{r}) = \exp\left[-\frac{i}{\hbar v} \int_{-\infty}^{\infty} dz\, \hat{V}(\mathbf{b},z,\mathbf{r}) \right]. \tag{9}$$

In Eqs. (7)–(9) the quantities ψ_α and ψ_0 are the wave functions of the excited and ground states of an atom, dependent on the $3Z_2$ coordinates of the atomic electrons $\mathbf{r} = (\mathbf{r}_1,\mathbf{r}_2 \ldots,\mathbf{r}_{z_2})$. Integration in Eq. (7) is carried out over the phase volume $d\tau = d\mathbf{r}_1 d\mathbf{r}_2 \ldots d\mathbf{r}_{z_2}$; $V(\mathbf{b},\mathbf{r})$ is the potential of the interaction between a passing particle and an atom. Substituting Eqs. (7)–(9) into Eq. (6) and allowing for completeness of the wave functions in a continuous spectrum as well as for the sum rule of the oscillator strengths, we obtain

$$\left(\frac{dE}{dx}\right)_I = N_0 \frac{2\pi}{kk_0} \int_{q_0}^{q_m} q\, dq \int d\tau\, d\tau'\, \psi_0^*(\mathbf{r}')\, G^*(\mathbf{r}',\mathbf{q})\, G(\mathbf{r},\mathbf{q})\, \psi_0(\mathbf{r}) \times [\hat{H}(\mathbf{r}) - E_0]\, \delta(\mathbf{r} - \mathbf{r}'), \tag{10}$$

where

$$\hat{H}(\mathbf{r}) = -\frac{\hbar^2}{2m}\sum_{i=1}^{Z_2}\nabla_{\mathbf{r}_i} + \hat{W}(\mathbf{r})$$

is the Hamiltonian operator of the atoms. After integration in Eq. (10) with respect to the set of variables $\mathbf{r}'$ and simple transformations, we obtain

$$\left(\frac{dE}{dx}\right)_I = \frac{N_0\hbar^2}{4\pi m}\sum_{i=1}^{Z_2}\int_{q_0}^{q_m} q\,dq\int d\tau\,|\psi_0(\mathbf{r})|^2 \times\left|\int d\mathbf{b}\exp(i\mathbf{qb})\nabla_{\mathbf{r}_i}\Gamma(\mathbf{b},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_2})\right|^2. \quad (11)$$

The summation in Eq. (11) is over the coordinates of all the electrons of the target atom. In the case of Eq. (5), the integration is with respect to small values of the transferred momentum $\mathbf{q}$, i.e., in a region defined by $qa_0 \ll 1$. The small values of q correspond to the case when a heavy particle moves in such a way that the impact parameter of an atom is large. The perturbation of an atom by a particle flying past is small and the phase interaction function can be expanded as a series in terms of a small parameter $\hat{V}(|\mathbf{b}| \gg a_0, z, \mathbf{r})/E_p$, where E_p is the kinetic energy of a heavy particle. If in this expansion we limit ourselves to the first two terms, we find that

$$\Gamma(\mathbf{b},\mathbf{r}) = 1 - \frac{i}{\hbar v}\int_{-\infty}^{\infty} dz\,\hat{V}(\mathbf{b},z,\mathbf{r}). \quad (12)$$

Using the approximation of Eq. (12), we find that the inelastic scattering amplitude considered in the Glauber–Franco approximation is identical with the amplitude of the first Born approximation. Using perturbation theories[29,30] in the dipole approximation, we can write down directly the expression for the energy losses due to the excitation of an atom:

$$\left(\frac{dE}{dx}\right)_a = \frac{4\pi e^4}{mv^2} Z_2 \ln\left(\frac{\varepsilon_I}{I_z}\right), \quad (13)$$

where I_z is the average ionization energy defined in terms of the oscillator strength $F_{0\alpha}$ for transitions from the ground to an excited state (described by the set of quantum numbers α):

$$Z_2 \ln(I_z) = \sum_{\alpha} \ln(E_\alpha - E_0) F_{0\alpha}, \quad (14)$$

where ε_I is the energy of an electron in the I th state.

The oscillator strength is described by

$$F_{0\alpha} = \frac{2m}{(e\hbar)^2}(E_\alpha - E_0)\,|d_{0\alpha}|^2, \quad (15)$$

where $d_{0\alpha}$ is a matrix element of the dipole moment of an atom (assumed to be nonzero). In the investigated range of velocities of a heavy charged particle $\varepsilon_I/I_z \approx 1$ and later we shall ignore the contribution due to the energy losses as a result of transitions in a discrete spectrum, valid to within logarithmic accuracy).

It follows from Eq. (11) that in this approach the energy losses depend on the distribution of the electron density of an atom, i.e., the approach allows for the individual features of the occupancy of the electron shells and it is not assumed that the interaction with the individual atomic electrons is statistically independent, i.e., it is not assumed that dE/dx is proportional to Z_2, but an allowance is made for a more complicated dependence. It is shown in Ref. 31 that when the proton velocity v is comparable with the average velocity of atomic electrons v_e, the greatest contribution to the energy losses comes from electrons in the outer shells of the target atom. When the condition $v \gg v_e$ is satisfied, the contribution to the energy losses made by each of the shells is approximately the same and the energy losses are proportional to the number of electrons.

3. BETHE-BLOCH RELATIONSHIP AND THE MODEL OF LOCAL OSCILLATORS

The interaction between an atom with Z_2 electrons and a passing proton is described by the sum of the Coulomb interactions between the proton and the nucleus and electrons:

$$\hat{V}(\mathbf{R},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_2}) = \frac{Z_2 e^2}{R} - \sum_{i=1}^{Z_2}\frac{e^2}{|\mathbf{R}-\mathbf{r}_i|}, \quad (16)$$

where $\mathbf{r}_i$ are the electron coordinates and $\mathbf{R}$ is the proton coordinate. Substituting Eq. (16) into Eq. (9) and integrating over the longitudinal coordinate, we find that the phase interaction function is[32]

$$\Gamma(\mathbf{b},\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{Z_2}) = 1 - \prod_{j=1}^{Z_2}\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{b}\right)^{2i\lambda}, \quad (17)$$

where $\lambda = v_0/v$ is the ratio of the electron velocity in the first Bohr orbit to the velocity of the passing particle; $\mathbf{s}_j$ are the projections of the electron coordinates on a plane perpendicular to the direction of motion of the heavy particle. We can follow the interaction between the proton and many atomic electrons by representing the many-electron phase function of Eq. (17) as a combination of one-electron functions:

$$\Gamma(\mathbf{b},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_2}) = \sum_{i=1}^{Z_2}\Gamma_0(\mathbf{b},\mathbf{r}_i) - \sum_i\sum_{j<i}\Gamma_0(\mathbf{b},\mathbf{r}_i)\Gamma_0(\mathbf{b},\mathbf{r}_j) + \sum_i\sum_{j<i}\sum_{j<k}\Gamma_0(\mathbf{b},\mathbf{r}_i)\Gamma_0(\mathbf{b},\mathbf{r}_j)\Gamma_0(\mathbf{b},\mathbf{r}_k) - \ldots, \quad (18)$$

where the one-particle phase function Γ_0 is of the form

$$\Gamma_0(\mathbf{b},\mathbf{r}) = 1 - \left(\frac{|\mathbf{b}-\mathbf{s}|}{b}\right)^{2i\lambda}. \quad (19)$$

We can interpret Eq. (18) as follows: the first term represents the contribution of the scattering by Z_2 electrons, which is statistically independent because of individual interactions between the passing particle and the individual electrons of the target atoms; the second term is the contribution of double interactions with different electron pairs, and so on. If the condition

$$\lambda Z_2 \ll 1 \quad (20)$$

is satisfied, the main contribution comes from the first term in Eq. (18). The condition (20) is identical with the condition for the validity of the first Born approximation and shows that if we go beyond this approximation, we can allow for the process of the scattering of the heavy particle by atomic electrons (see Ref. 32).

We also assume that the scattering phase is acquired

because of the single-interaction processes, i.e.,

$$\Gamma(\mathbf{b}, \mathbf{r}_1, \ldots, \mathbf{r}_{Z_2}) \approx \sum_{i=1}^{Z_2} \Gamma_0(\mathbf{b}, \mathbf{r}_i). \tag{21}$$

The hypothesis corresponding to Eq. (21) imposes limitations on the proton velocity, which should be greater than the average velocity of atomic electrons. We assume that in this approximation the total phase is simply the sum of the single-particle phases and we should denote by $\rho_j(\mathbf{r})$ the density of the electron distribution in the jth shell. This gives

$$\frac{dE}{dx} = \frac{N_0\hbar^2}{4\pi m} \sum_j n_j \int_{q_j}^{q_{max}} q\, dq \int d\mathbf{r}\, \rho_j(\mathbf{r}) \times \int d\mathbf{b} \exp(i\mathbf{qb}) \,|\, \nabla_r \Gamma_0(\mathbf{b}, \mathbf{r}) \,|^2. \tag{22}$$

The summation in Eq. (22) is carried out over all the filled shells of an atom: n_j is the number of electrons in the jth shell ($\Sigma n_j = Z_2$).

We obtain the asymptotic expression for the energy losses in the limit of high proton velocities. If the condition $\lambda \ll 1$ is satisfied, the one-particle phase function (19) is of the form

$$\Gamma_0(\mathbf{b}, \mathbf{r}) \approx -2i\lambda \ln\left(\frac{|\mathbf{b}-\mathbf{s}|}{b}\right), \tag{23}$$

whereas the integral over the impact parameter $\mathbf{b}$ of the gradient with respect to the electron position is

$$\int d\mathbf{b} \exp(i\mathbf{qb})\, \nabla_r \Gamma_0(\mathbf{b}, \mathbf{r}) = \frac{4\pi i\lambda \mathbf{q}}{q^2} \exp(i\mathbf{qs}). \tag{24}$$

Substituting Eq. (24) into Eq. (22) and integrating over the transferred momentum, we obtain

$$\frac{dE}{dx} = \frac{4\pi N_0 \hbar^2 \lambda^2}{m} \sum n_j \int d\mathbf{r}\, \rho_j(\mathbf{r}) \ln\left(\frac{2mv^2}{I_j}\right), \tag{25}$$

where I_j is the energy of an electron in the jth shell of the target atom.

If we introduce the average energy through

$$\ln I_z = \frac{1}{Z_2} \sum_j n_j \ln I_j, \tag{26}$$

which is independent of the position of the atomic electrons (see Ref. 29), we obtain—as expected—the Bethe–Bloch relationship, Eq. (1). It is clear from Eq. (25) that if the condition $\lambda \ll 1$ is satisfied, the contribution made to the total losses by electrons from different shells is the same (to logarithmic accuracy) and the atomic electrons can be regarded as free.

If we assume that each element of the atomic volume is characterized by a frequency ω, which is related to the local density of the electron gas by

$$\omega^2 = \gamma_0 4\pi e^4 \rho(\mathbf{r})/m, \tag{27}$$

where γ_0 is a constant of the order of unity,[33] then in this model the value of I_j represents the excitation energy of an electron located at a point with the coordinate $\mathbf{r}$, i.e., $I_j = \hbar\omega(\mathbf{r})$, and instead of Eq. (26) we now have

$$Z_2 \ln(I_z) = 4\pi \int r^2\, dr \ln[\hbar\omega(\mathbf{r})]\rho(\mathbf{r}). \tag{28}$$

If we assume that at low values of the argument ($x \ll 1$) the modified Bessel function $K_0(x)$ obeys an approximate relation

$$K_0(x) \approx \ln\left[\frac{2}{x}\exp(-C)\right], \tag{29}$$

where C is Euler's constant, we find that the energy losses considered subject to Eqs. (27)–(29) can be now expressed in the form

$$\frac{dE}{dx} = \frac{4\pi N_0 \hbar^2 \lambda^2}{m} Z_2 \int d\mathbf{r}\, \rho(\mathbf{r}) K_0\left(\frac{\alpha\hbar\omega(\mathbf{r})}{mv^2}\right), \tag{30}$$

where $\alpha \approx 0.56$.

Equation (30) was derived in Ref. 20 using the local-oscillator model. In this model a moving particle creates a spatial charge distribution characterized by the frequency ω. The electric field resulting from the space charge decelerates the moving particle. Calculations of the spatial distribution of the charge[20,34] show that it depends weakly (logarithmically) on the density of the electron distribution in the target atoms and the induced charges themselves are located near the path of the passing particle in a certain finite region of radius R_0, which is a free parameter in the theory and is found by comparing the results of calculations of the energy losses with the experimental data.

4. ENERGY LOSSES EXPERIENCED BY PROTONS IN HYDROGEN AND HELIUM TARGETS: NUCLEAR DYNAMIC SHADOW

We use Eq. (22) to calculate the energy losses due to the excitation and ionization of atoms in hydrogen and helium targets. The distribution of the electron density of a hydrogen atom in the ground state is

$$\rho(r) = \frac{1}{\pi a_0^3} \exp\left(-\frac{2r}{a_0}\right). \tag{31}$$

Substituting Eq. (31) into Eq. (22) and integrating with respect to the longitudinal coordinate of an electron and with respect to the angular variables, we obtain

$$\frac{dE}{dx} = \frac{16\pi N_0 \hbar^2 \lambda^4}{m} \int_{a_0 q_1}^{a_0 q_{max}} t\, dt \int_0^\infty dx\, x^4 K_1(2x)\, W(\lambda t x), \tag{32}$$

where

$$W(z) = [K_0^2(z) + K_1^2(z)]\, I_0(2z) - 2K_0(z)K_1(z)I_1(2z), \tag{33}$$

$K_0(z)$ and $K_1(z)$ are modified functions of the second kind, and $I_0(z)$ and $I_1(z)$ are modified Bessel functions of the first kind. At small values of the argument $z \to 0$ in Eq. (33) we find that $W(z) \to z^{-2}$ and then Eq. (32), subject to the condition $\lambda \ll 1$, yields the Bethe–Bloch relationship (1) for the energy losses in a hydrogen target. Curve 1 in Fig. 1 gives the results of calculations of the energy lost by protons, carried out using Eqs. (31)–(33). For comparison, it also includes the results of calculations based on Eq. (1) (curve 2) and the data of Ref. 16. The energy losses of protons in targets made of practically all the elements are presented in a systematic manner in Ref. 16. According to Ref. 16, the errors in the values of the energy losses represent less than 1% in the case of protons with energies exceeding 400 keV, and can reach 10% at lower energies. Subsequently published measure-

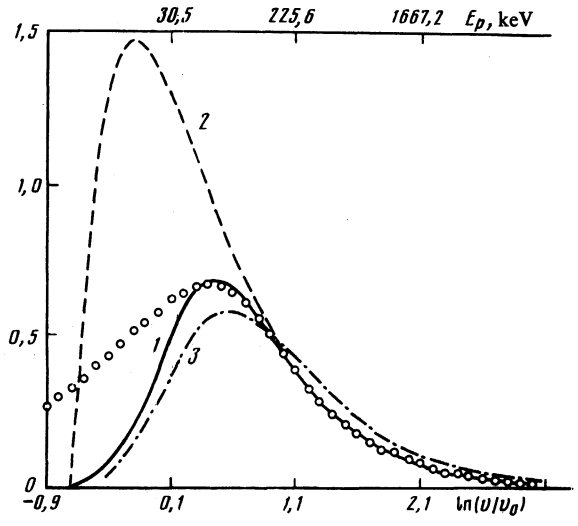

FIG. 1. Energy losses experienced by protons in a hydrogen target [the ordinate gives the dimensionless quantity $(m/4\pi\hbar^2 N_0)dE/dx$]: 1) calculations carried out using Eqs. (31)–(33); 2) calculations carried out using the Bethe–Bloch relationship (1); 3) calculations carried out assuming the delta-like electron density distribution; O) data taken from Ref. 16.

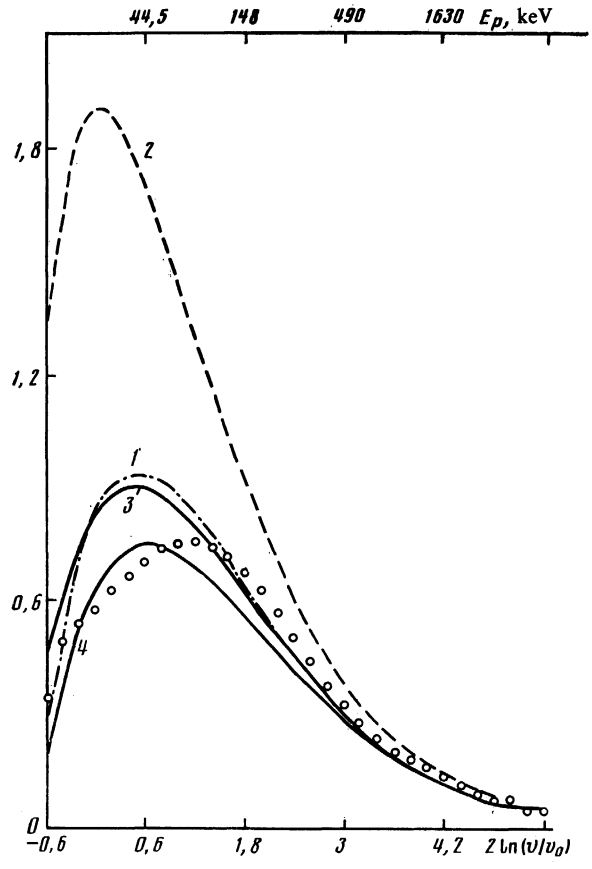

FIG. 2. Energy losses experienced by protons in a helium target (the ordinate gives the same quantity as in Fig. 1): 1) calculated ignoring multiple collisions; 2) calculated using the Bethe–Bloch relationship; 3) ortho-helium target (allowing for multiple collisions); 4) para-helium target (allowing for multiple collisions); O) data taken from Ref. 16.

ments of the losses[35,36] are in good agreement with the data of Ref. 16. We can see from Fig. 1 that some differences between the results of calculations and the experimental data of Ref. 16 at low proton energies are due to neglect of the electron exchange process.

We now consider how the distribution of the electron density affects the energy losses. As an example we take the distribution of the electron density in the form of a Dirac δ-function. This exactly localized choice implies that the electron is at a distance a_0 from a nucleus. Curve 3 in Fig. 1 gives the results of calculations of the losses for this particular distribution. It is clear from this figure that in the region of the maximum of the curve the energy losses depend strongly on the nature of the distribution. As the energy of the passing particle is increased, the losses become less and less sensitive to the nature of the distribution and in the range of validity of the Born approximation they are practically independent of the distribution, which is the reason why the Bethe–Bloch relationship is universally valid.

The next element in the periodic system is the He atom. Its ground state has the $1s^2$ configuration, where both electrons are in the $1s$ state and the radial part of the wave function is symmetric under coordinate transposition:

$$\Psi_{\mathrm{He}}(\mathbf{r}_1\mathbf{r}_2)=\psi_{1s}(\mathbf{r}_1)\psi_{1s}(\mathbf{r}_2). \qquad (34)$$

We select ψ_{1s} hydrogen-like functions with the effective charge parameters deduced from a variational principle.[12] The results of calculations of the energy losses experienced by protons in a He target are presented in Fig. 2. For comparison, this figure includes also the results of Ref. 16 and the calculations carried out using the Bethe–Bloch expression.

We can see from Figs. 1 and 2 that the energy losses calculated from Eq. (22) agree better with the experimental data than calculations carried out using the Bethe–Bloch expression. The reason for this agreement is that, as shown in Ref. 32, the scattering becomes weaker if we go beyond the perturbation theory framework. This weakening is because the Glauber–Franco approximation we have used for the inelastic scattering amplitude allows for the elastic interaction between the incident particle and the nucleus. This interaction can alter the initial direction of motion of a particle so it passes an atomic electron at distances such that energy transfer to the electron is impossible, i.e., the electron is in the dynamic shadow of the nucleus and is practically uninvolved in the elastic interaction with the particle.

We now consider the characteristic size of this shadow region. Deceleration of a heavy particle due to the interaction with a single electron depends on the displacement of this electron in an atom during the collision time. If this displacement is small compared with the characteristic period of the electron motion, then the binding forces have no significant influence on the energy transfer process. In the opposite case of a long collision time the atom can be regarded as experiencing a static field of forces. Then its state remains the same after a collision. Consequently, the binding forces limit from above the effective impact parameter within which the transfer of energy to bound electrons is still possible.

A collision characterized by an impact parameter b lasts for a time of order b/v, which should not exceed the characteristic atomic period ω^{-1}, i.e., we should have $b_{\max} \approx v/\omega$. The motion of a particle carried by the maxi-

mum impact parameter corresponds to the minimum possible transferred momentum. Consequently, the motion of a particle at distances $b > b_{max}$ from the nucleus should not result in its deceleration. The interaction of a particle with an electron at a distance R_a from a nucleus is characterized by the impact parameter $b + \theta R_a$, where $\theta \ll 1$ is the angle of deviation of the particle from the direction of its initial motion. Allowing for the relationship between the impact parameter and the scattering angle (in the Coulomb interaction case) given by $\theta \approx 2Z_2e^2/Mv^2b$ (Ref. 12), we find that the interaction between a heavy particle and an electron occurs at distances b exceeding the critical value

$$b_c = 2(Z_2e^2R_a/E)^{1/2}, \tag{35}$$

which is the minimum possible distance in the particle–(nucleus)–electron system. If the condition $b_c \geqslant b_{max}$ is satisfied, electrons which at the moment of interaction are in the rear hemisphere of the atom cannot contribute to the energy losses, i.e., they are in the dynamic shadow of the nucleus. We can rewrite Eq. (35) in a more convenient form

$$b_c = Z_2^{2/3}(v_0/v)R_a. \tag{36}$$

It follows from Eq. (36) that the characteristic size of the shadow region depends strongly on the velocity of the particle. For $b_c < R_a$ the particle interacts with all the electrons in the atom and the influence of the nucleus on the inelastic scattering process is slight. The condition $b \ll R_a$ is identical with the condition for the validity of the Born approximation in which the influence of a nucleus on the inelastic scattering process is ignored.[29]

Turning back to Figs. 1 and 2, it should be pointed out that the greatest difference between the results of calculations carried out using Eqs. (1) and (22) occurs for slow protons in the region of the maximum of the loss curve. In this region the electrons of a target atom are in the dynamic shadow of the nucleus and this weakens the inelastic scattering and reduces the energy losses. Moreover, in this region the losses depend strongly on the distribution of electrons in the target atoms.

We illustrate this by the example of calculation of protons decelerating in an ortho-helium target. The lowest state of ortho-helium has the configuration $1s2s$ with the spin $S = 1$ and the radial part of the wave function is antisymmetric under electron coordinate transposition. The results of calculations carried out using Eq. (22) ignoring a slight reduction in the losses due to the process of transfer of a helium atom to the ground state are shown in Fig. 2 (curve 3). It is clear from Fig. 2 that near the maximum of the curve the losses in para-helium are approximately 40% less than in ortho-helium. This can be explained by the fact that the average radius of the He atom in the $1s2s$ state is approximately twice as large as in the $1s^2$ state, i.e., one of the electrons is almost outside the region of the dynamic shadow of the nucleus and it interacts effectively with the passing particle, which results in its strong deceleration. Since the ionization energy is less for ortho-helium than for para-helium, the process of momentum transfer begins at a lower proton energy and a maximum of the curve shifts toward lower velocities. When the proton velocity is increased, the dynamic shadow region becomes smaller [see Eq. (36)], some of the electrons are outside the shadow, and the energy losses are given by the Bethe–Bloch expression (1).

In comparing the results of calculations with the data of Ref. 16 we can see (Fig. 2) that there is a considerable discrepancy in the region of the maximum of the loss curve. The discrepancy is due to the fact that Eq. (22) ignores the scattering by different atomic electrons, i.e., only the first term in the expansion of the phase function of Eq. (18) is included. We can allow for this effect by applying the exact expression (15) to the ground state of a two-electron atom

$$\frac{dE}{dx} = \frac{N_0\hbar^2}{4\pi m}\int_{q_1}^{q_{max}} q\,dq \int d\mathbf{r}_1\,d\mathbf{r}_2\,\rho(\mathbf{r}_1,\mathbf{r}_2)$$
$$\times\left\{\left|\int d\mathbf{b}\exp(i\mathbf{qb})\,\nabla_{\mathbf{r}_1}\Gamma_0(\mathbf{b},\mathbf{r}_1)\,[1-\Gamma_0(\mathbf{b},\mathbf{r}_2)]\right|^2 + \left|\int d\mathbf{b}\exp(i\mathbf{qb})\,\nabla_{\mathbf{r}_2}\Gamma_0(\mathbf{b},\mathbf{r}_2)\,[1-\Gamma_0(\mathbf{b},\mathbf{r}_1)]\right|^2\right\}. \tag{37}$$

We interpret Eq. (37) as an expression describing the energy lost by a proton due to its interaction with the "first electron" when it is partially dynamically shadowed by the nucleus, allowing for the possibility of simultaneous scattering by the "second" electron [represented by the first term in the braces of Eq. (37)]. A similar situation occurs also in the case of the "second" electron (represented by the second term). It follows from the principle of indistinguishability of electrons that the contributions by the first and second terms are identical. The results of calculations of the energy lost by protons described by the wave function of Eq. (34) are presented in Fig. 2 (curve 2). It is clear from this figure that the agreement between the calculations and the data of Ref. 16 is now much better.

5. CONCLUSIONS

The quantum-mechanical approach and the Glauber–Franco approximation for the inelastic scattering amplitude were used to analyze the energy losses due to the processes of excitation and ionization of atoms in an amorphous target when it interacts with a heavy particle characterized by a unit charge. The results obtained without the use of empirical and fitting parameters ensure good agreement with the experimental data. An analysis of the reasons for such an agreement shows that the influence of the elastic nuclear scattering channel is important near the maximum of the dependence of the losses on the velocity of a heavy particle. The deviation of the heavy particle from its initial direction, due to the Coulomb interaction with the nucleus, means that it may travel at such distances relative to an electron of a target atom that the transfer of energy to this electron is impossible, i.e., the electron is in the dynamic shadow created by the nucleus and in practice does not participate in the interaction with the passing particle. An estimate of the characteristic size of the shadow region shows that it is inversely proportional to the velocity of this particle.

In the case of slow particles (in the region of the maximum of the loss curve) the influence of the dynamic shadow results in significant weakening of the inelastic scattering and reduces the losses, in agreement with the experimental results. In the case of fast particles the shadow region is small and the energy losses are given by the classical Bethe–Bloch expression. In addition to the dynamic shadow, the process of deceleration of a particle flying past is influenced also by

multiple scattering by electrons in the same atom. Calculations indicate that the contribution of this process is 10–15% in the case of slow particles and its inclusion improves the agreement with the experimental data.

The proposed model is invalid in the case of very slow particles whose velocity is much less than the average velocity of atomic electrons, because it ignores perturbation of the wave function of the target atom and deceleration due to the exchange of electrons between the colliding particles.

The nuclear dynamic shadow effects in multiple electron scattering effects must be taken into account in determining how the effective charge of a moving particle affects its velocity, and also in analyses of the dependence of the energy losses on Z_1 and Z_2.

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