

- factorily described within the framework of the simple model of the effective free ion. In this case effects not accounted for in the one-center self-consistent calculation influence strongly the XCS.^{14,15}
- ²The less rigorous procedure used in Ref. 19 to reduce the experimental results led to a noticeable systematic underestimate of the XCS.
- ¹G. J. Perlow and M. R. Perlow, *J. Chem. Phys.* **48**, 955 (1968). G. J. Perlow, in: *Chemical Application of Mössbauer Spectroscopy*, ed. V. I. Goldanskii and R. H. Herber, Acad. Press, N.Y., 1968, p. 376.
- ²J. C. Hindman and A. Svirmickas, in: *Noble Gas Compounds*, ed. by H. H. Hyman, Univ. Chicago Press, Chicago, 1963, p. 251.
- ³G. J. Jameson and H. S. Gutowsky, *J. Chem. Phys.* **40**, 2285 (1964).
- ⁴D. Ladzins, C. W. Kern, and M. Karplus, *J. Chem. Phys.* **39**, 1611 (1963).
- ⁵J. R. Morton and W. E. Falconer, *J. Chem. Phys.* **39**, 427 (1963).
- ⁶H. Basch, J. W. Moskowitz, C. Hollester, and D. Hankin, *J. Chem. Phys.* **55**, 1922 (1971).
- ⁷T. X. Carrol, R. W. Shaw, T. D. Thomas, C. Kindle, and N. Bartlett, *J. Am. Chem. Soc.* **96**, 1989 (1974).
- ⁸L. B. Barinskiĭ and V. I. Nefedov, *Rentgeno-spektral'noe opredelenie zaryada atomov v molekulakh (x-ray Spectral Determination of the Charge of Atoms in Molecules)*, Nauka, Moscow, 1966, Chap. 1.
- ⁹J. Hinze and K. S. Pitzer, in: *Noble Gas Compounds*, ed. by H. H. Hyman, Univ. Chicago Press, Chicago, 1963, p. 340.
- ¹⁰C. A. Coulson, *J. Chem. Soc.* 1442 (1964).
- ¹¹J. G. Malm, H. Selig, J. Jortner, and S. A. Rice, *Chem. Rev.* **65**, 199 (1965).
- ¹²M. A. Ratner and J. R. Sabin, *J. Am. Chem. Soc.* **99**, 3954 (1977).
- ¹³M. E. Dyatkina and N. M. Klimenko, *Zh. Strukt. Khim.* **14**, 173 (1973).
- ¹⁴E. V. Petrovich, Yu. P. Smirnov, V. S. Zykov, A. I. Grushko, O. I. Sumbaev, I. M. Band, and M. B. Trzhaskovskaya, *Zh. Eksp. Teor. Fiz.* **61**, 1756 (1971) [*Sov. Phys. JETP* **34**, 935 (1971)].
- ¹⁵M. A. Coulthard, *J. Phys. B* **7**, 440 (1974).
- ¹⁶L. I. Molkanov, Yu. S. Grushko, I. M. Band, G. A. Shadrina, and M. B. Trzhaskovskaya, *Zh. Eksp. Teor. Fiz.* **70**, 2218 (1976) [*Sov. Phys. JETP* **43**, 1158 (1976)]. Yu. S. Grushko, L. I. Molkanov, I. M. Band, and A. V. Oleinik, *Usp. Fiz. Nauk* **113**, 362 (1974) [*Sov. Phys. Usp.* **17**, 464 (1974)].
- ¹⁷V. I. Nefedov, *Zh. Strukt. Khim.* **8**, 1037 (1967).
- ¹⁸I. M. Band and M. B. Trzhaskovskaya, Preprint No. 92, Leningrad Inst. Acad. Sci., 1974.
- ¹⁹I. S. Kirin, Yu. K. Gusev, V. K. Isupov, L. I. Molkanov, V. Ya. Mishin, and A. V. Krupinskaya, *Zh. Neorg. Khim.* **16**, 2916 (1971).
- ²⁰V. Ya. Mishin, I. S. Kirin, V. K. Isupov, and Yu. K. Gusev, *Zh. Neorg. Khim.* **16**, 51 (1971).
- ²¹T. M. Spittler and B. Jaselskis, *J. Am. Chem. Soc.* **87**, 3357 (1965); J. G. Malm and E. H. Appelman, *At. Energ. Rev.* **7**, 3 (1969).
- ²²V. I. Goldanskii and E. F. Makarov, in: *Chemical Application of Mössbauer Spectroscopy*, ed. by V. I. Goldanskii and R. H. Herber, Acad. Press, N.Y., 1968.
- ²³S. L. Ruby and G. K. Shenoy, *Phys. Rev.* **186**, 326 (1969).
- ²⁴H. de Waard, in: *Mössbauer Effect Data Index*, ed. by J. G. Stevens and V. E. Stevens, IFI/Plenum, N.Y., Washington, 1975, p. 447.
- ²⁵C. A. Coulson, *Valence*, Oxford Univ. Press, London, 1961.
- ²⁶R. Latter, *Phys. Rev.* **99**, 510 (1955).
- ²⁷D. S. Urch, *J. Inorg. Chem.* **25**, 771 (1963).
- ²⁸O. P. Charkin, A. E. Smolyar, A. S. Zyubin, and N. M. Klimenko, *Zh. Strukt. Khim.* **15**, 539 (1974).
- ²⁹P. S. Bagus, B. Liu, D. H. Liskow, and H. F. Schäfer, *J. Am. Chem. Soc.* **97**, 7216 (1975).

Translated by J. G. Adashko

Coulomb excitation of atoms by fast protons

V. A. Ryabov and G. L. Yudin

(Submitted 13 June 1979; resubmitted 27 September 1979)
Zh. Eksp. Teor. Fiz. **78**, 474-484 (February 1980)

A Green's function technique is developed for calculating the dependence of the energy loss of heavy charged particles on the impact parameter in the quasiclassical approximation. Formulas are derived for the probabilities of bound-bound transitions in hydrogenlike atoms, and for their asymptotic values in the dipole approximation and in the strong coupling approximation. Simpler expressions than those previously derived are obtained for bound-free transitions. An analysis of the contributions of various Coulomb excitation channels is carried out on the basis of the results. An exact calculation of the energy losses shows that the mean-frequency approximation is not valid for the inner shell electrons.

PACS numbers: 34.10. + x, 34.50.Hc

1. INTRODUCTION

Originally, interest in processes of Coulomb excitation of atoms arose in the study of energy losses of fast electrons, protons and alpha particles in the medium. The corresponding quantum theory was constructed by Bethe.¹ It is applicable in the case in which the ratio of the velocity of the electron in the atom v_0 to the velocity of the incoming particle

$$\xi = v_0/v = \hbar/mv = Z_0 e^2/\hbar v \quad (1)$$

is much less than unity (m is the mass of the electron, Z_0 is the charge of the nucleus of the target atom).

In collisions with the participation of heavy particles ($M \gg m$), the deBroglie wavelength \hbar/Mv is, as a rule much less than the characteristic atomic dimensions $1/\lambda$. This allows us to assume the trajectory of the incoming particle to be classical, and to consider the ex-

citation of the atom as the result of the interaction of the electron with a moving force center.

The classical approach, which is not connected with the requirement $\xi \ll 1$, has been widely used for calculations of total and partial cross sections of the various excitation channels. However, in recent years, a whole series of problems have arisen in the physics of atomic collisions, in which the dependence of the excitation of atoms on the value of the impact parameter is isolated in explicit fashion. The possibility of the experimental study of a similar dependence is connected either with the inhomogeneity in the spatial distribution of the flux of incoming particles, as is the case, for example, in channeling,² or with the observation of single collisions. The latter is realized in experiments on the scattering of atomic beams by thin films and gases. Here the impact parameter is determined from the angle of deflection of the incoming particle, and the excitation channel is identified by the characteristic radiation with the help of a coincidence technique.

In most experimental researches,³⁻⁷ the dependence on the impact parameter of the total probability of ionization of the atomic shells is studied. There are also data relating to bound-bound transitions in hydrogen and helium.^{8,9} Theoretical calculations of the ionization probability as a function of the impact parameter have been carried out in the well-known work of Bang and Hans-teen¹⁰ (see also Refs. 11 and 12) and bound-bound transitions between separate shells have been investigated in Ref. 13.

The problem of the dependence of the probability of the different excitation channels on the impact parameter has paramount importance for the analysis of the channeling effect. We are dealing with the calculation of that part of the energy loss of channeled particles that is connected with Coulomb excitation of the atoms of a single crystal. The calculation of the dependence of the energy losses on the impact parameter has not been completely carried out at the present time. Only the ionization part of the energy losses has been investigated. In the calculations of the bound-bound transitions, the difficulty due to the necessity of summation of the excitation probability over degenerate finite states has not been overcome.

In a number of researches¹⁴⁻¹⁷ they used for the calculation of the energy losses of channeled particles the mean frequency approximation, which allows us to carry out summation in the formula for the losses over all the intermediate states. In particular, quantitative calculation of the dependence of the energy losses on the impact parameter over the entire region of its variation was first carried out in Ref. 15. It is not possible to estimate the limits of applicability of the mean-frequency approximation in the absence of accurate results without mentioning the fact that in the framework of such an approximation, let alone the fact that in this approximation it is not possible to pose the question of the relative contributions to the losses in the individual excitation channels.

A quasiclassical method of treatment of the effects of

Coulomb excitation is developed in the present work. It is based on the use of the Green's function of the target atom. This method allows us to calculate accurately, from a single point of view, the dependence on the impact parameter both in the energy losses and in the probabilities of individual transitions in the discrete and continuous spectra. We also emphasize that when using the Green's function, summation of the transition probabilities over the degenerate finite states is carried out automatically. The formulas used below for the probabilities of bound-bound transitions make it possible to carry out a systematic analysis of the dependence of the total energy losses on the impact parameter. We also note that the expressions for the probabilities of bound-free transitions, found with the help of the Green's function, is much simpler than that previously known.¹⁰

2. GENERAL RELATIONS

We shall assume that the incoming particle moves along a classical trajectory $\mathbf{R}(t)$, while the time-dependent potential of its interaction with each electron of the target atom, $\hat{V}(t)$, produces transitions between different states in the atom. The amplitudes of these transitions are equal, in first order in $\hat{V}(t)$, to¹¹

$$\mathfrak{M}_{fi}(\mathbf{b}) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt \exp[i(\omega_f - \omega_i)t] \langle f | \hat{V}(t) | i \rangle. \quad (2)$$

Because of the excitation of the atom, the incoming particle loses an energy equal to the transition energy $\hbar(\omega_f - \omega_i)$.

The energy losses of a fast-charged particle are determined by the following quantities:

$$\Delta^l E(b) = \sum_f (\hbar\omega_f - \hbar\omega_i)^l |\mathfrak{M}_{fi}|^2, \quad l=1,2, \quad (3)$$

$\Delta^1 E$ is the effective retardation of the particle per atom, $\Delta^2 E$ is the broadening of the energy spectrum (straggling).

We shall assume that the origin of the coordinates is chosen at the center of the target atom, and the trajectory is rectilinear:

$$\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t. \quad (4)$$

The velocity vector of the incoming particle \mathbf{v} is constant and directed along the z axis, while the impact parameter \mathbf{b} lies in the xy plane.

Choosing the interaction potential in the form of a retarded Coulomb potential,

$$\hat{V}(t) = -\frac{Ze^2}{2\pi^2} \int \frac{d^3q}{q^2 - (\mathbf{q}\mathbf{v}/c)^2} \exp[i(\mathbf{q}\mathbf{r} - \mathbf{q}\mathbf{b} - \mathbf{q}\mathbf{v}t)], \quad (5)$$

we write the amplitude of the transition (2) in the form

$$\mathfrak{M}_{fi}(\mathbf{b}) = \frac{i}{\pi} \left(\frac{Ze^2}{\hbar v} \right) \int \frac{d^3q}{q^2 - (\mathbf{q}\mathbf{v}/c)^2} \delta \left(q_z - \frac{\omega_f - \omega_i}{v} \right) e^{-i\mathbf{q}\mathbf{b}} \langle f | e^{i\mathbf{q}\mathbf{r}} | i \rangle. \quad (6)$$

The mean-frequency approximation, about which we spoke in the Introduction, consists in the replacement of $(\omega_f - \omega_i)$ in the argument of the δ function in (6) by some value $\bar{\omega}$. In such a substitution, the losses (3) are easily calculated with the help of the sum rule.¹⁵

Taking the result (6) into account, we can transform the expression for the energy losses, separating out the

coordinate dependence of the wave functions of the final state $|f\rangle = \psi_f(\mathbf{r})$. The partition function that arises in this case is itself the imaginary part of the Green's function of the unperturbed atom:

$$G(\mathbf{r}_2, \mathbf{r}_1; \omega) = \sum_s \frac{\psi_s^*(\mathbf{r}_1) \psi_s(\mathbf{r}_2)}{\omega - \omega_s + i0}. \quad (7)$$

The final result of the transformation is conveniently represented in the following form:

$$\Delta' E(\mathbf{b}) = -\frac{1}{\pi^2} \left(\frac{Ze^2}{\hbar v} \right)^2 \hbar^2 v^{l+1} \iint \frac{d^3 q_1 d^3 q_2}{[q_1^2 - (\mathbf{q}\mathbf{v}/c)^2] [q_2^2 - (\mathbf{q}\mathbf{v}/c)^2]} \times q_z \delta(q_{1z} - q_{2z}) \text{Im} \{ e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{b}} J(\mathbf{q}_1, \mathbf{q}_2) \}, \quad (8)$$

where

$$J(\mathbf{q}_1, \mathbf{q}_2) = \iint d^3 p_1 d^3 p_2 \psi_i(\mathbf{p}_1 - \mathbf{q}_1) G(\mathbf{p}_2, \mathbf{p}_1; q_z v + \omega_i) \psi_f^*(\mathbf{p}_2 - \mathbf{q}_2). \quad (9)$$

Formulas (8) and (9) establish the connection between the energy losses and the convolution of the Green's function, written in the momentum representation, with respect to the initial state.

Further calculations are possible only for a specific model of the target atom. We shall limit ourselves below to consideration of a hydrogen-like atom with effective nuclear charge Z_a .

The integral representation for the Coulomb Green's function was obtained by Schwinger¹⁸ (see also Refs. 19 and 20):

$$G(\mathbf{p}_2, \mathbf{p}_1; \omega) = -\frac{mp^2}{2\pi^2 \hbar} \left(\frac{i \exp(i\pi\lambda/p)}{2 \sin(\pi\lambda/p)} \right)^{(0+)} \int_1^{(0+)} dz z^{-\lambda/p} \times \frac{d}{dz} \left\{ \frac{1-z^2}{z} \left[p^2 (\mathbf{p}_1 - \mathbf{p}_2)^2 + (p_1^2 + p_2^2) (p_2^2 + p^2) \frac{(1-z)^2}{4z} \right]^{-2} \right\}, \quad (10)$$

$$p^2 = -2m(\omega + i0)/\hbar, \quad \text{Re } p > 0.$$

The contour of integration in (10) is taken along a unit circle from $z = 1 + i0$ to $z = i0$.

Carrying out the integration over the momenta in the expression for $J(\mathbf{q}_1, \mathbf{q}_2)$, after substitution there of the Green's function (10) and the wave function of the K electron,

$$\psi_{1s}(\mathbf{q}) = \pi^{-1} (8\lambda^3)^{-1/2} (q^2 + \lambda^2)^{-2} \quad (11)$$

(the mathematical details of the method of integration are set forth in Refs. 19 and 20), we find

$$J(\mathbf{q}_1, \mathbf{q}_2) = -\frac{16}{\hbar} m\lambda^3 p \left(\frac{i \exp(i\pi\lambda/p)}{2 \sin(\pi\lambda/p)} \right) \times \int_1^{(0+)} dz z^{-\lambda/p} \frac{\partial^2}{\partial \lambda_1 \partial \lambda_2} (A_1 z^2 - 2Bz + A_2)^{-1} \Big|_{\lambda_1 = \lambda_2} \quad (12)$$

$$A_{1,2} = [(p \mp \lambda_1)^2 + q_1^2] [(p \mp \lambda_2)^2 + q_2^2], \quad (13)$$

$$B = 4p^2 (\mathbf{q}_1 \mathbf{q}_2) + (\lambda_1^2 + q_1^2 - p^2) (\lambda_2^2 + q_2^2 - p^2). \quad (14)$$

The transition cross sections and the energy losses integrated over the impact parameters are determined from the following formulas:

$$\sigma_{fi} = \int d^2 b |\mathfrak{M}_{fi}(\mathbf{b})|^2 = 4 \left(\frac{Ze^2}{\hbar v} \right)^2 \int \frac{d^2 q}{[q^2 - (\mathbf{q}\mathbf{v}/c)^2]^2} \times \delta \left(q_z - \frac{\omega_f - \omega_i}{v} \right) |\langle f | e^{i\mathbf{q}\cdot\mathbf{r}} | i \rangle|^2, \quad (15)$$

$$\Delta' E = -\frac{4}{\pi} \left(\frac{Ze^2}{\hbar v} \right)^2 \hbar^2 v^{l+1} \int \frac{d^2 q}{[q^2 - (\mathbf{q}\mathbf{v}/c)^2]^2} q_z^2 \text{Im} \{ J(\mathbf{q}, \mathbf{q}) \}. \quad (16)$$

For the hydrogen-like atom,

$$J(\mathbf{q}, \mathbf{q}) = -\frac{64}{\hbar} m\lambda^3 p \left(\frac{i \exp(i\pi\lambda/p)}{2 \sin(\pi\lambda/p)} \right) \int_1^{(0+)} dz z^{-\lambda/p} \frac{z^2 (\lambda - p)^2 - 2z(\lambda^2 - 2p^2) + (\lambda + p)^2}{\{z[(\lambda - p)^2 + q^2] - [(\lambda + p)^2 + q^2]\}^2}. \quad (17)$$

We note that integration over the longitudinal momentum q_z is equivalent to summation over the excited states. The real and imaginary values of the parameter p in formula (10) correspond respectively to the bound-bound and bound-free transitions of an electron in an atom. As a consequence of the symmetry $J(\mathbf{q}_1, \mathbf{q}) = J(\mathbf{q}_2, \mathbf{q}_1)$, the energy losses on an atom of hydrogen are expressed only by $\text{Im} J(\mathbf{q}_1, \mathbf{q}_2)$. The procedure of calculation of $\text{Im} J(\mathbf{q}_1, \mathbf{q}_2)$ requires special attention, since poles in the expressions (12)–(14) in the case of excitation of states of discrete and continuous spectra have a different origin. For this reason, the contributions of the bound-bound and bound-free transitions is considered separately.

3. BOUND-BOUND TRANSITIONS

According to formula (6), the amplitude \mathfrak{M}_{fi} is expressed in terms of the formfactor $\langle f | e^{i\mathbf{q}\cdot\mathbf{r}} | i \rangle$, the value of which is well known for transitions of any type in the hydrogen atom.²¹ Therefore, the principal difficulty in finding the probabilities of bound-bound transitions lies in the necessity of summation of the squares of the moduli of the amplitudes (6) over the degenerate final states. In the Green's function method, such a summation is carried out automatically, because, upon separation of the imaginary part the only poles that make a contribution to (8)–(9) correspond to the energy spectrum of the scattering system.

We can establish the fact that the imaginary part of $J(\mathbf{q}_1, \mathbf{q}_2)$ in the case of a hydrogen atom is determined by the singularity of the factor in curly brackets in front of the contour integral in (12):

$$\text{Im} J(\mathbf{q}_1, \mathbf{q}_2) \sim \text{Im} \frac{1}{\sin(\pi\lambda/p - i0)} = \pi \sum_n (-1)^n \delta \left(\frac{\lambda}{p} - n \right), \quad (18)$$

$$p = (\lambda^2 - 2mq_z v)^{1/2}.$$

The result of integration over the admissible values of q_z ($0 < q_z < \lambda^2/2mv$) is represented in the form

$$\Delta' E(\mathbf{b}) = \left(\frac{\hbar^2 \lambda^2}{2m} \right)^l \sum_{n=2}^{\infty} \left(1 - \frac{1}{n^2} \right)^l W_n(\mathbf{b}); \quad (19)$$

$W_n(\mathbf{b})$ is the probability of excitation with transition of the electron from the K shell ($n=1$) to an arbitrary state $|n\rangle$. For transitions into a state of the discrete spectrum, the roots of the square of the trinomial in the denominator of the integrand of (12) are complex and less than unity in modulus. Consequently, the function in front of the contour integral in $W_n(\mathbf{b})$ has no other singularities than a pole of the n -th order at the point $z=0$. Therefore, the contour can be closed at the point $z=1$ and the theorem of residues applied to the calculation of the integral. As a result, we find:

$$W_n(\mathbf{b}) = \frac{16}{\pi^2 n^4} \left(\frac{Ze^2}{\hbar v} \right)^2 \iint \frac{d^2 Q_1 d^2 Q_2}{(Q_1^2 + \eta^2/\gamma^2) (Q_2^2 + \eta^2/\gamma^2)} \times e^{i(\mathbf{Q}_1 - \mathbf{Q}_2) \cdot \mathbf{b}} \frac{\partial^2}{\partial \mu_1 \partial \mu_2} \left(\frac{\sin n\Phi}{\sin \Phi} \frac{A_1^{(n-1)/2}}{A_2^{(n+1)/2}} \right) \Big|_{\mu_{1,2}=1}. \quad (20)$$

$$A_{1,2} = \left[\left(\frac{1}{n} \mp \mu_1 \right)^2 + Q_1^2 + \eta^2 \right] \left[\left(\frac{1}{n} \mp \mu_2 \right)^2 + Q_2^2 + \eta^2 \right], \quad (21)$$

$$B = \frac{4}{n^2} (Q_1 Q_2 + \eta^2) + \left(\mu_1^2 + Q_1^2 + \eta^2 - \frac{1}{n^2} \right) \left(\mu_2^2 + Q_2^2 + \eta^2 - \frac{1}{n^2} \right), \quad (22)$$

$$\Phi = \arctg \left(\frac{A_1 A_2}{B^2} - 1 \right)^{1/2}, \quad \eta = \frac{\xi}{2} \left(1 - \frac{1}{n^2} \right). \quad (23)$$

Here and everywhere below, the impact parameter b is measured in units of $1/\lambda$, and $\gamma = (1 - v^2/c^2)^{-1/2}$ is the Lorentz factor.

Since further simplification of formulas (20)–(23) without any limitation is not possible, we turn to the asymptotic estimates for several important special cases. Thus, for excitation channels accompanied by transitions between inner shells ($\xi \gg 1, \gamma = 1$), the integrand in (20) can be factorized in terms of the variables Q_1 and Q_2 and calculation gives

$$W_n(b) \approx \frac{16}{n^2} \left(\frac{Ze^2}{\hbar v} \right)^2 \left(\frac{b}{\eta} \right)^4 [K_n(b\eta)]^2, \quad (24)$$

$K_n(x)$ is the modified Bessel function.

Integration over $Q_{1,2}$ is materially simplified in the case of valence electrons ($\xi \ll 1$) at large impact parameters ($b \gg 1$), i.e., in the dipole approximation. The basic contribution to the integral is made by values of $Q_{1,2} \ll 1$; therefore,

$$W_n(b) \approx \frac{2^{10}}{3n^2} \left(\frac{Ze^2}{\hbar v} \right)^2 \eta^2 \frac{(1-1/n)^{2n-5}}{(1+1/n)^{2n+5}} \times \left\{ \left[K_0 \left(\frac{b\eta}{\gamma} \right) \right]^2 + \left[\frac{1}{\gamma} K_1 \left(\frac{b\eta}{\gamma} \right) \right]^2 \right\}. \quad (25)$$

In conclusion, we give the results of the solution of the problem of the cross section of the Coulomb excitation process. It is simplest to obtain it not by turning to the general formulas (20)–(23), but by starting out from the relations (16) and (17). All the integrals in this case are evaluated analytically. Thus, at $\gamma = 1$,

$$\sigma_n = -\frac{2^8 \pi}{\lambda^2} \left(\frac{Ze^2}{\hbar v} \right)^2 \left\{ \frac{4}{3n^2} \frac{A^{2n-5}}{B^{2n+5}} \ln \left(1 + \frac{4}{\xi^2 A^2} \right) + \frac{1}{n^2 B^{10}} \left[B^2 \left(\frac{n+2}{n-1} \right) F_{n-1} + 2(1-2AB) \left(\frac{n+1}{n-2} \right) F_{n-2} + A^2 \left(\frac{n}{n-3} \right) F_{n-3} \right] \right\}, \quad (26)$$

$$F_m = \sum_{r=0}^m \binom{m}{r} \left(\frac{A^2}{B^2} - 1 \right)^r \sum_{s=r}^{r+4} \binom{r+4}{s} \frac{(-1)^s}{1-s} \times \left[\left(1 + \frac{4}{\xi^2 A^2} \right)^{1-s} - 1 \right], \quad (27)$$

$$A = 1 - 1/n, \quad B = 1 + 1/n.$$

In the limits $\xi \ll 1$, the formula for the cross section was first obtained by Bethe¹ by direct calculation of the matrix elements in the expression (15).

4. BOUND-FREE TRANSITIONS

Although, just as in the case of bound-bound transitions, the imaginary part of the function $J(q_1, q_2)$ is determined by the infinitesimally small increment to the expression for p^2 , for the ionization channels it does not contain any singularities. The integrand in (12) has poles at points corresponding to the roots of the square of the trinomial. Transforming from contour integration to angle integration ($z = e^{i\psi}$) and substituting in (12)–(14)

the quantity

$$p = -i(2mq_2 v - \lambda^2)^{1/2} = -i\lambda k, \quad (28)$$

we obtain

$$\text{Im } J(q_1, q_2) = \frac{8m\lambda^8 k}{1 - \exp(2\pi/k)} \times \int_0^{2\pi} d\psi e^{\nu/k} \frac{\partial^2}{\partial \lambda_1 \partial \lambda_2} \text{Im} \frac{1}{|A| \cos(\varphi - \psi) - B + i0} \Big|_{\alpha_{1,2} = \lambda}, \quad (29)$$

$$A_1 = |A| \exp(-i\varphi).$$

The choice of the sign in the right side of (28) is determined by the requirement $\text{Re } p > 0$ [see (10)]. The delta functions in (29) make it possible to carry out integration over the angle ψ in a simple way.

The ionization part of the energy loss (8) can be represented in the form

$$\Delta' E''(b) = \left(\frac{\hbar^2 \lambda^2}{2m} \right)^2 \int_0^\infty dk (k^2 + 1)^2 \left(\frac{dW(b)}{dk} \right). \quad (30)$$

Here the probability of emission of an electron with momentum $\hbar \lambda k$, obtained with account of the relation (29), is equal to

$$\frac{dW(b)}{dk} = \frac{32}{\pi^2} \left(\frac{Ze^2}{\hbar v} \right)^2 \frac{k^2}{1 - e^{-2\pi/k}} \times \iint \frac{d^2 Q_1 d^2 Q_2}{(Q_1^2 + \eta^2/\gamma^2)(Q_2^2 + \eta^2/\gamma^2)} e^{i(Q_2 - Q_1) \cdot b} \times \frac{\partial^2}{\partial \mu_1 \partial \mu_2} \frac{e^{\nu/k}}{(|A|^2 - B^2)^{1/2}} \text{ch} \left(\frac{1}{k} \arccos \frac{B}{|A|} \right) \Big|_{\nu_{1,2} = -1}, \quad (31)$$

$$A = [(ik + \mu_1)^2 + Q_1^2 + \eta^2] \times [(ik + \mu_2)^2 + Q_2^2 + \eta^2] = |A| e^{-i\varphi}, \quad (32)$$

$$B = -4k^2 (Q_1 Q_2 + \eta^2) + (\mu_1^2 + Q_1^2 + \eta^2 + k^2)(\mu_2^2 + Q_2^2 + \eta^2 + k^2), \quad (33)$$

$$\eta = \xi(k^2 + 1)/2. \quad (34)$$

Numerical calculations of the dependence of the ionization probability on the impact parameter have been carried out in a number of works (see, for example, Refs. 10, 12, 22). It must be emphasized that the formula (31) is much simpler than the widely used formula introduced by Bang and Hansteen.¹⁰ It contains essentially a triple integral over the transverse transferred momenta and the angle between them.

By analogy with the results of the previous section, we write down the analytic expressions for the probability of ionization in two limiting cases. For excitation channels accompanied by transitions of strongly bound electrons, and also in the case of large transferred momenta ($\eta \gg k + 1, \gamma = 1$),

$$\frac{dW(b)}{dk} \approx \left(\frac{Ze^2}{\hbar v} \right)^2 \frac{16k}{1 - e^{-2\pi/k}} \left(\frac{b}{\eta} \right)^4 [K_2(b\eta)]^2. \quad (35)$$

In the dipole approximation ($b \gg 1$) at not too large transfers of the momentum to the weakly bound electron ($\eta \ll k + 1$),

$$\frac{dW(b)}{dk} \approx \frac{2^{10}}{3} \left(\frac{Ze^2}{\hbar v} \right)^2 \frac{k}{1 - e^{-2\pi/k}} \exp \left\{ -\frac{2}{k} \text{Arctg} \left(\frac{2k}{1 - k^2} \right) \right\} \times \frac{\eta^2}{(k^2 + 1)^2} \left\{ \left[K_0 \left(\frac{b\eta}{\gamma} \right) \right]^2 + \left[\frac{1}{\gamma} K_1 \left(\frac{b\eta}{\gamma} \right) \right]^2 \right\}, \quad (36)$$

$$\text{Arctg } x = \begin{cases} \arctg x, & \text{if } x \geq 0 \\ \pi + \arctg x, & \text{if } x < 0 \end{cases}$$

As also in the case of bound-bound electrons, the use of the expression for $J(\mathbf{q}, \mathbf{q})$ (17) at $\gamma=1$ leads immediately to the formula for the ionization cross section²:

$$\frac{d\sigma}{dk} = \frac{2^{10}\pi}{3\lambda^2} \left(\frac{Ze^2}{\hbar v}\right)^2 \frac{k}{1-\exp(-2\pi/k)} \int_0^\infty \frac{dx}{x} \frac{3x+1+k^2}{[(x+1-k^2)^2+4k^2]^{3/2}} \times \exp\left\{-\frac{2}{k} \text{Arctg}\left(\frac{2k}{x+1-k^2}\right)\right\}. \quad (37)$$

5. DISCUSSION OF THE RESULTS

We now turn to the general formula for the bound-bound transitions (20)–(23) at $\gamma=1$. In the initial portion [$b(\xi+1) \ll 1$], the probabilities $W_n(\mathbf{b})$ do not depend on the value of the impact parameter. With increase in b they fall off first according to a power law and then (at $b \gg 1$) according to an exponential one. In the special case $\xi=1$, this is confirmed by the numerical calculations represented in Fig. 1. In this drawing the curve of the total ionization probability is also shown.²² It is seen that the probability of excitation of states of discrete and continuous spectra are quantities of the same order.

Figure 2 shows the dependence of the effective stopping power on the impact parameter in the case of strong and weak coupling of the electron in the atom. For comparison, the results of calculations in the mean-frequency approximation are also given.¹⁵ We note that whereas the error involved in the mean frequency approximation is relatively small in the region $\xi \ll 1$, the approximation results for the electrons of the inner shells can depart from the exact ones by several orders of magnitude. This is clear since the value of $\bar{\omega}$ was determined in Ref. 15 from a comparison of the effective stopping power integrated over the impact parameters, with the Bethe formula, which is valid only at $\xi \ll 1$. The energy losses behave in nonmonotonic fashion with increase in ξ . At small ξ they increase, at $\xi \approx 1$ the losses are maximal and upon further increase in ξ they fall off rapidly.

In the limit $b \rightarrow 0$ our calculations give results that are too high, since we have completely neglected the distortion of the real trajectory of the incoming particle because of its interaction of the target atom with the nucleus. Nevertheless, the point $b=0$ is of interest as a tie-in point of the monotonically decreasing (with in-

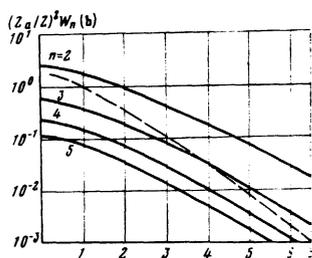


FIG. 1. Dependence of the probabilities of the separate channels of Coulomb excitation of the atom on the impact parameter. ($\xi=1$, $\gamma=1$). The dashed curve is the total ionization probability. The continuous curves are the probabilities of bound-bound transitions. The impact parameter is measured in units of $1/\lambda$.

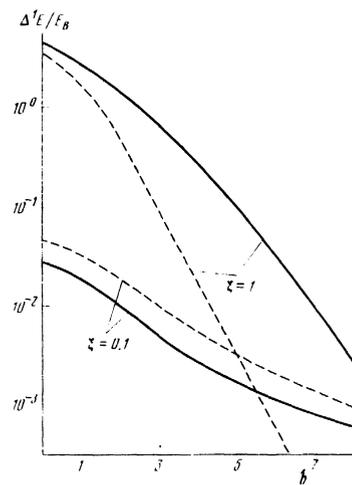


FIG. 2. Dependence of the effective stopping power per atom on the impact parameter ($\gamma=1$). $E_B = \lambda^2/2mZ_a^2$. The continuous curves are the exact results. The dashed curves are calculated in the mean frequency approximation.¹⁵ The impact parameter is measured in units of $1/\lambda$.

crease in the impact parameter) transition probabilities. The dependences of the probabilities of the separate channels of excitation on ξ at $b=0$ are shown in Fig. 3. The curve for the total ionization probability is obtained by extrapolation of the data given in Ref. 22. It is seen from Fig. 3 that the relative contribution of the ionization part of the energy loss falls off rapidly with increase in ξ . This circumstance takes place also at arbitrary impact parameters.

At first glance it may seem that the Green's function method, developed in the present paper, is applicable only in the approximation of rectilinear trajectories. However, this is not the case. At $\gamma=1$, the δ function, which leads finally to the imaginary part of the Green's function, also appears in expression (2) for arbitrary form of the quasi-classical trajectories $\mathbf{R}(t)$. It is simplest to separate it by expanding the interaction potential $V(t)$ into a Fourier integral in the time. Then the Fourier components of the energy losses will be determined by the formulas (8) and (9).

The allowance for the relativistic effects reduces to the fact that the dependence of the probabilities of Coulomb excitation on the impact parameter changes significantly with increase in the Lorentz factor γ . In the range of values $b\xi \ll \gamma$ the time of flight of the proton

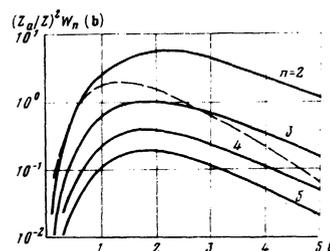


FIG. 3. Probabilities of the separate excitation channels at $b=0$ as a function of the parameter ξ ($\gamma=1$). The dashed curve is the total ionization probability. The continuous curves are the probabilities of bound-bound transitions.

past the atom is much less than the characteristic times of atomic transitions. At $v \sim c$ in the range $b \leq 1$ the transition probabilities do not depend on the impact parameter. The role of relativistic effects at $b \gg 1$ reduces, generally speaking, to the appearance of the scale factor $1/\gamma$ in front of the impact parameter b , as is seen from the expressions (25) and (26). This circumstance also leads to the experimentally observed logarithmic increase in the cross sections ($\sim \ln \gamma^2$) (see, for example, Ref. 23).

For light atomic targets, the limitations connected with the use of the quasiclassical approach and the choice of a definite trajectory of the impinging heavy particle reduce to the satisfaction of the inequality $\gamma m \ll M$ ($E \ll 10^3 \text{ GeV/nucleon}$). The latter means that the maximum energy transferred in a collision with a free electron at rest, $2\gamma^2 m v^2$, is much less than the energy of the particle $\gamma M c^2$.

The region of applicability of the approximation of rectilinear trajectories at $\xi \leq 1$ is extraordinarily large: $bM\gamma \gg \xi^2 m$. For electrons of the inner shells ($\xi \gg 1$), when the transition probabilities are exponentially small in view of the adiabatic character of the excitation, an insignificant change in the classical trajectory of the impinging particle can affect substantially the value of the excitation probability. Correspondingly, the conditions of application of the approximation of rectilinear trajectories becomes more severe: $\xi^3 \ll M/m$.

A strict account of the spin effects in the cross sections of Coulomb excitation of heavy atom targets on the basis of numerical solutions of the Dirac equation has appeared recently.^{24, 25}

In conclusion, a few words on the use of the results obtained in this research for the analysis of the energy losses of channeled particles. Although the losses take place in the crystal and not in hydrogen-like atoms, our results and the results of Refs. 15, 16 are the first and necessary step in the quantitative estimate of the energy losses in localized electrons. The difficulty of the problem is such that at this very day, the hydrogen-like model used by us is the only one that admits of a complete calculation, which was carried out for the first time in this paper.

We thank O. B. Firsov and V. A. Bazylev for useful discussions of the described results.

¹For our problem, the criterion of applicability of perturbation theory is the inequality $\min(Z/Z_a, Ze^2/\hbar v) \ll 1$.

- ¹H. A. Bethe, *Ann. Phys.* **5**, 325 (1930).
²D. S. Gemmell, *Revs. Mod. Phys.* **46**, 129 (1974).
³J. U. Andersen, L. Kocbach, E. Laegsgaard, M. Lund, and C. D. Moak, *J. Phys.* **B9**, 3247 (1976).
⁴J. E. Chemin, S. Andriamonje, S. Denagbe, J. Poturier, B. Saboya, and J. P. Thibaud, *Phys. Rev.* **A15**, 1851 (1977).
⁵K. H. Weber and F. Bell, *Phys. Rev.* **A16**, 1075 (1977).
⁶H. Schmidt-Böcking, R. Schule, K. E. Stiebing, K. Bethge, I. Tserruya, and H. Zekl, *J. Phys.* **B10**, 2663 (1977).
⁷B. M. Johnson, K. W. Jones, W. Brandt, F. C. Jundt, G. Guillaume, and T. H. Kruse, *Phys. Rev.* **A19**, 81 (1979).
⁸J. T. Park, J. M. George, J. L. Peacher, and J. E. Aldag, *Phys. Rev.* **A18**, 48 (1978).
⁹J. T. Park, J. E. Aldag, J. L. Peacher, and J. M. George, *Phys. Rev. Lett.* **40**, 1646 (1978).
¹⁰J. Bang and J. M. Hansteen, *Mat. Fyz. Medd. Dan. Vid. Selsk.* **31**, No. 13 (1959).
¹¹J. M. Hansteen and O. P. Mosebekk, *Nucl. Phys.* **A201**, 541 (1973).
¹²L. Kocbach, *J. Phys.* **B9**, 2269 (1976).
¹³D. R. Bates, *Proc. Roy. Soc. (London)* **245**, 299 (1958); J. Van den Bos and F. J. de Heer, *Physica* **34**, 333 (1967).
¹⁴M. Kitagawa and Y. H. Ohtsuki, *Phys. Rev.* **B5**, 3418 (1972).
¹⁵K. Dettmann and M. T. Robinson, *Phys. Rev.* **B10**, 1 (1974).
¹⁶K. Dettmann, *Z. Physik* **A272**, 227 (1975).
¹⁷Yu. Kagan and Yu. V. Kononets, *Zh. Eksp. Teor. Fiz.* **66**, 1693 (1974) [*Sov. Phys. JETP* **39**, 832 (1974)].
¹⁸J. Schwinger, *J. Math. Phys.* **5**, 1606 (1964).
¹⁹M. Gavrila and A. Costescu, *Phys. Rev.* **A2**, 1752 (1976).
²⁰M. Gavrila, *Phys. Rev.* **A6**, 1348 (1972).
²¹A. O. Barut and R. Wilson, *Phys. Rev.* **A13**, 918 (1976).
²²J. M. Hansteen, O. M. Johnson, and L. Kocbach, *Atom. Data Nucl. Data Tables* **15**, 305 (1975).
²³V. S. Asoskov, V. V. Blazhenkov, V. M. Grishin, V. K. Ermilova, L. P. Kotenko, G. I. Merzon, and P. S. Pervov, *Zh. Eksp. Teor. Fiz.* **76**, 1274 (1979) [*Sov. Phys. JETP* **49**, 646 (1979)].
²⁴D. M. Davidović, B. L. Moiseiwitsch, and P. N. Norrington, *J. Phys.* **B11**, 847 (1978).
²⁵R. Anholt, *Phys. Rev.* **A19**, 1004 (1979).

Translated by R. Beyer