Excitation of multiply charged ions by electron impact

L. P. Presnyakov and A. M. Urnov

P. N. Lebedev Physics Institute, USSR Academy of Sciences
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The system of strong-coupling integral equations is solved for the problem of excitation of an ion of charge $Z \gg 1$ by electron impact. The representation used for the radial Green's function of the Coulomb field permits construction of a solution in the form of a proper expansion in the small parameter Z^{-1}. The asymptotically exact expression for the scattering matrix contains two terms which respectively describe potential and resonance scattering. It is shown that coupling of the open channels leads to small corrections in the parameter Z^{-1} to the potential scattering. In the cross section averaged over the resonances, the contribution of the resonance term corresponding to strong coupling with the closed channels has the same order of magnitude as potential scattering, and in a number of cases it is dominant. As an illustration we present the results of numerical calculations of the cross sections for excitation of a number of transitions in the lithiumlike ion of oxygen.

1. In the scattering of electrons by positively charged ions, the attractive Coulomb field leads to characteristic features in the cross sections near the thresholds of new (energetically closed) channels (see ref. 1), the cause of which is the formation and decay of quasistationary states of the system ion + electron (so-called resonance scattering). Baz'[2] established the existence of near-threshold resonance structure and jumps in the elastic cross sections. Gaĭlitis[3] and Seaton[4] obtained a generalization of the results of Baz'[2] to the case of inelastic processes. In refs. 1–4 the analytic properties of the scattering matrix have been investigated in the immediate vicinity of the threshold of the new channel. Use of the results of refs. 3 and 4 for calculation of the cross sections for excitation of ions by electron impact requires, however, solution of the strong-coupling equations, i.e., reduces to another extremely complex problem.[5] Therefore the question of the quantitative contribution of resonance scattering to the cross section and consequently of the accuracy of methods not taking it into account, which is characteristic of most applications, remains open to a significant degree.

In the problem of excitation of multiply charged ions by electron impact, the small parameter Z^{-1} naturally arises, where (Z−1) is the charge of the ion. This permits construction of a solution of the many-channel problem in the form of an asymptotic series in powers of Z^{-1}. In the present work a proper expansion has been obtained on the basis of the approach developed by Feshbach.[6,7] The representation used by us for the Green's function of the Coulomb field permits separation in explicit form of the effects of resonance scattering, which provide a contribution to the cross section of the same order in the parameter Z^{-1} as direct (potential) scattering.

2. We will proceed from the system of radial strong-coupling equations written in Coulomb units:

$$\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+\frac{2a}{r}+k_\Gamma^2\right\}F_\Gamma=\frac{1}{Z}\sum_{\Gamma'}U_{\Gamma\Gamma'}F_{\Gamma'}. \tag{1}$$

Here $Z = Z_n - N + 1$, where Z_n is the charge of the nucleus and N is the number of electrons of the ion, $a = 1-Z^{-1}$, Γ is the complete set of quantum numbers of the channel, and l is the orbital angular momentum of the outer electron. In the general case the potentials $U_{\Gamma\Gamma'}$ are integral operators and are expressed in terms of radial integrals (see ref. 8). It is important that for $Z \gg 1$ all $U_{\Gamma\Gamma'}$ are practically independent of Z.

We will rewrite the system (1) in integral form, separating the open channels ($\Gamma = \alpha$) and the closed channels ($\Gamma = \beta$):

$$F_\alpha=\delta_{\alpha\Gamma_0}P_{\Gamma_0}+\frac{1}{Z}\sum_{\Gamma}\hat{G}_\alpha^{(+)}U_{\alpha\Gamma}F_\Gamma, \tag{2}$$

$$F_\beta=\frac{1}{Z}\sum_{\Gamma}\hat{G}_\beta^{(+)}U_{\beta\Gamma}F_\Gamma. \tag{3}$$

The function P_{Γ_0} is the regular solution of the homogeneous equation (1) for the entrance channel. The kernels of the integral operators are the Coulomb Green's functions $G_k^{(+)}(r, r')$ which correspond to the scattering problem. We will define the momentum of the channel in the upper half-plane of the k plane by the expression

$$k_\Gamma=\sqrt{2(E-\Delta E_{\Gamma\Gamma_0})},\quad \operatorname{Im} k_\Gamma\geqslant 0, \tag{4}$$

where E and $\Delta E_{\Gamma\Gamma_0}$ are respectively the total energy and excitation energy of the level Γ.

In contrast to the problem of excitation of a neutral atom, in the case $Z > 1$ the coupling of the open channels is weak. From formal expansion of F_α in perturbation theory in the small parameter Z^{-1}, it is evident that in the absence of closed channels the n-th term of the series falls off as $\sim Z^{-n}$. Thus, inclusion of only open channels gives small corrections to the first-order perturbation theory. We note that the question of first-order perturbation theory—the so-called Born-Coulomb approximation and its modifications for inclusion of exchange—has been discussed in detail by Beĭgman and Vaĭnshteĭn.[9,10]

In the presence of even one closed channel, there arise in each term of the perturbation-theory expansion, beginning with the second, resonance denominators corresponding to the poles of the Coulomb Green's function, in the vicinity of which special consideration is necessary. We will represent the Green's function in the form of two terms, separating the part which is the main one in energy, which has a pole and a point of crowding of poles at the threshold of each closed channel. After a number of identical transformations we obtain for $G_k^{(+)}(r, r')$ an expression valid for the physical sheet of $E-\Delta E_{\Gamma\Gamma_0}$:

$$G_k^{(+)}(r,r')=\frac{\pi\nu^3}{2a^2}\operatorname{ctg}(\pi\nu)P_{\nu,l}(r)P_{\nu,l}(r')+G_k^{(p)}(r,r'), \quad (5)$$

$$G_k^{(p)}(r,r')=\frac{\pi\nu^3}{2a^2}\frac{P_{\nu,l}(r_<)}{\sin(\pi\mu)}[\cos(2\pi\mu)P_{\nu,l}(r_>)-P_{\nu,-l-1}(r_>)], \quad (6)$$

$$\mu\to l+\frac{1}{2}, \quad \nu=\frac{ia}{k}, \quad \operatorname{Im}k\geqslant 0. \quad (7)$$

The functions $P_{\nu,l}$ for $\nu = n (n = 1, 2, 3, \ldots)$ coincide with the radial eigenfunctions $P_{n,l}$ of the discrete spectrum of the problem of motion in a Coulomb field and are related to the functions $P_{k,l}$ of the continuum by the expression

$$P_{\nu,l}(r)=C_\nu P_{kl}(r), \quad \nu=ia/k, \quad (8)$$

$$C_\nu=\left\{\frac{2a^2}{\pi\nu^2[i\operatorname{ctg}(\pi\nu)+1]}\right\}^{1/2}, \quad (9)$$

which are valid for all ν defined by Eq. (7).

Factorization of the first term in Eq. (5) in the variables r and r′ permits accurate inclusion of the contribution of the pole part in the energy dependence of the solutions of the system (2) and (3). Separating in the right-hand part of (3) the term corresponding to the Green's function $G_k^{(p)}$ regular in k (and independent of k as $k \to 0$), we rewrite the system (2) and (3) in the form

$$F_\alpha=\delta_{\alpha\Gamma_0}P_{\Gamma_0}+\frac{1}{Z}\sum_\Gamma \hat{G}_\alpha^{(+)}U_{\alpha\Gamma}F_\Gamma, \quad (10)$$

$$F_\beta=P_\beta\Lambda_\beta+\frac{1}{Z}\sum_\Gamma \hat{G}_\beta^{(p)}U_{\beta\Gamma}F_\Gamma, \quad (11)$$

where the quantities Λ_β, which do not depend on the coordinates, are given by

$$\Lambda_\beta=\frac{\pi\nu^3}{2a^2}\operatorname{ctg}(\pi\nu)\sum_\Gamma\langle P_\beta U_{\beta\Gamma}F_\Gamma\rangle. \quad (12)$$

Here and subsequently we use the designations

$$P_\alpha=P_{k_\alpha,l}(r), \quad P_\beta=C_{\nu_\beta}P_{k_\beta,l}(r). \quad (13)$$

For $\nu \neq n$, Eqs. (10) and (11) with regular kernels can be formally integrated by the iteration method. Their solutions are expressed in terms of the quantities Λ_β as follows:

$$F_\alpha=\delta_{\alpha\Gamma_0}P_{\Gamma_0}+\frac{1}{Z}\hat{G}_\alpha^{(+)}W_{\alpha\Gamma_0}P_{\Gamma_0}+\frac{1}{Z}\sum_\beta\hat{G}_\alpha^{(+)}W_{\alpha\beta}P_\beta\Lambda_\beta, \quad (14)$$

$$F_\beta=P_\beta\Lambda_\beta+\frac{1}{Z}\hat{G}_\beta^{(p)}W_{\beta\Gamma_0}P_{\Gamma_0}+\frac{1}{Z}\sum_{\beta'}\hat{G}_\beta^{(p)}W_{\beta\beta'}P_{\beta'}\Lambda_{\beta'}. \quad (15)$$

When Eq. (12) is taken into account, the quantities Λ_β are solutions of the algebraic system of equations

$$\sum_{\beta'}\left[Z\frac{2a^2}{\pi\nu^3}\operatorname{tg}(\pi\nu)\delta_{\beta\beta'}-\langle P_\beta W_{\beta\beta'}P_{\beta'}\rangle\right]\Lambda_{\beta'}=\langle P_\beta W_{\beta\Gamma_0}P_{\Gamma_0}\rangle. \quad (16)$$

Equations (14)–(16) contain expansions in the small parameter Z^{-1}:

$$W_{\Gamma\Gamma'}=U_{\Gamma\Gamma'}+\sum_{\substack{n=1\\ i\leqslant n}}^{\infty}\frac{1}{Z^n}U_{\Gamma\Gamma_1}\hat{G}_{\Gamma_1}U_{\Gamma_1\Gamma_2}\ldots\hat{G}_{\Gamma_i}U_{\Gamma_i\Gamma'}. \quad (17)$$

In the series (17) we designate by $\hat{G}_\Gamma$ the quantity $\hat{G}_\alpha^{(+)}$ for $\Gamma = \alpha$ and $\hat{G}_\beta^{(p)}$ for $\Gamma = \beta$.

In contrast to standard perturbation theory, each term of the expansion used does not contain singularities in energy. The solutions of Eq. (15) are regular functions of the energy for all values of ν (see, for example, refs. 6 and 7). It should be noted that for complex k the integrals $\langle\ldots\rangle$ in Eq. (16) are usually calculated on the assumption of a finite range of interaction. However, this assumption can be avoided by changing the order of integration over the coordinates in these two integrals or by using the regularization procedure developed in refs. 1 and 11.

From the asymptote of Eq. (14), expressions for the T matrix of the open channels follow in an obvious manner:

$$T_{\alpha\Gamma_0}=T^p_{\alpha\Gamma_0}+T^r_{\alpha\Gamma_0}, \quad (18)$$

$$T_{\alpha\Gamma_0}=-\langle P_\alpha W_{\alpha\Gamma_0}P_{\Gamma_0}\rangle, \quad T^r_{\alpha\Gamma_0}=-\sum_\beta\langle P_\alpha W_{\alpha\beta}P_\beta\rangle\Lambda_\beta. \quad (18a)$$

The wave-function normalization used in the present work corresponds to a relation between the S and T matrices:

$$S=1+\frac{2i}{Z}T, \quad S_{\Gamma\Gamma_0}=\delta_{\Gamma\Gamma_0}+\frac{2i}{Z}T_{\Gamma\Gamma_0}. \quad (19)$$

The first term T^p in Eq. (18) is completely determined by the generalized potential $W_{\alpha\Gamma_0}$ given by the perturbation-theory series (17) with kernels $G_\alpha^{(+)}$ and $G_\beta^{(p)}$ which are regular in energy. The second term in Eq. (18), T^r, describes resonance scattering in the presence of a Coulomb field, due to the presence of closed channels, and is determined by the solution of the system of algebraic equations (16) for the quantities Λ_β. The summation in (16) is carried out over the set of quantum numbers β which characterize the closed channels.

In the case $Z \gg 1$ of interest here, it is sufficient to limit ourselves in the series (17) to the first nonvanishing terms for the real and imaginary parts of $W_{\Gamma\Gamma'}$. The element of the T matrix of potential scattering in this case is

$$T^p_{\alpha\Gamma_0}=-\langle P_\alpha U_{\alpha\Gamma_0}P_{\Gamma_0}\rangle=T^{(1)}_{\alpha\Gamma_0}, \quad (20)$$

i.e., it is identical with the element of the T matrix calculated in the first order of standard perturbation theory. It is easy to be convinced that, in the absence of accidental coincidence of resonances, the nondiagonal elements in the left part of (16) can be neglected, and the expression for $T^r_{\alpha\Gamma_0}$ will take the form

$$\left.\begin{aligned} T^r_{\alpha\Gamma_0}&=-\frac{1}{Z}\sum_\beta\frac{\tau_{\alpha\beta}(\nu_\beta)\tau_{\beta\Gamma_0}(\nu_\beta)}{\operatorname{tg}(\pi\nu_\beta)-Z^{-1}\tau_{\beta\beta}(\nu_\beta)+iZ^{-2}\Sigma_\beta},\\ \Sigma_\beta&=\sum_{\alpha'}\tau^2_{\beta\alpha'}(\nu_\beta),\end{aligned}\right\} \quad (21)$$

where $\tau_{\Gamma\beta}(\nu_\beta)$ is a real and symmetric matrix, diagonal in the closed channels:

$$\left.\begin{aligned} \tau_{\beta\beta'}&=\delta_{\beta\beta'}\left(\frac{\pi\nu_\beta^3}{2}\right)\langle P_\beta U_{\beta\beta}P_\beta\rangle,\\ \tau_{\alpha\beta}&=\tau_{\beta\alpha}=\left(\frac{\pi\nu_\beta^3}{2}\right)^{1/2}\langle P_\alpha U_{\alpha\beta}P_\beta\rangle.\end{aligned}\right\} \quad (22)$$

It should be noted that the energy dependence of $\tau(\nu)$ in Eqs. (21) and (22) is determined by the quantity $\nu_\beta = a[2(\Delta E_{\beta\alpha}-E_0)]^{-1/2}$, while in the region of existence of resonances ($\Delta E_{\alpha\Gamma_0} \leq E_0 \leq \Delta E_{\beta\alpha}$) $\nu_\beta \gg 1$ and τ is practically independent of energy. The value of τ^2 as $\nu \to \infty$ is related in an obvious manner[12] to the threshold value of the partial excitation cross section calculated in first-order perturbation theory. In the case of degeneracy of the ionic levels, it is necessary in obtaining τ to diagonalize the matrix $\langle P_\beta U_{\beta\beta'}P_{\beta'}\rangle$ in the

quantum numbers of the degeneracy.

Expression (21) is the sum of the contributions of all energetically inaccessible levels of the initial ion and describes the sequence of resonances which form the Coulomb crowding at the threshold of each such channel. This result is asymptotically exact for $Z \gg 1$ and arbitrary values of the incident-electron energy, and in the near-threshold regions, as we can easily see, it contains the known characteristic features.[3,4]

Let us determine the contribution of resonance scattering to the excitation cross section. The total cross section for excitation of a transition $\gamma_0 \to \gamma_1$ is determined by the relation

$$\sigma_{\gamma_0\gamma_1} = \sum_{l_0 l_1 \Gamma_T} \sigma_{\gamma_0 l_0, \gamma_1 l_1}, \tag{23}$$

where the partial cross section $\sigma_{\gamma_0 l_0,\ \gamma_1 l_1}$ is related to the element of the T matrix by the formula

$$\sigma_{\gamma_0 l_0, \gamma_1 l_1} = \frac{g(\Gamma_1)}{g(\gamma_0) Z^4 E_0} |T_{\Gamma_1 \Gamma_0}|^2 \pi a_0^2. \tag{24}$$

Here $g(\Gamma_1)$ and $g(\gamma_0)$ are the statistical weights of the states characterized by the sets of quantum numbers Γ_1 and γ_0. The sum in Eq. (24) is taken over the orbital quantum numbers l_0 and l_1, the total angular momenta, and the remaining intermediate quantum numbers entering into Γ.

The partial and total cross sections, as can be seen Eqs. (21) and (24), have sharp peaks, reaching values $\sim Z^2$ at the maximum and falling to a value σ^p depending smoothly on energy and determined by T^p. The final expression for the partial cross section, averaged over the resonances as in refs. 2–4, is of the form

$$\bar{\sigma}_{\gamma_0 l_0, \gamma_1 l_1} = \frac{1}{\Delta E} \int_{E-\Delta E}^{E+\Delta E} dE\, \sigma_{\gamma_0 l_0, \gamma_1 l_1} = \bar{\sigma}^p_{\gamma_0 l_0, \gamma_1 l_1} + \bar{\sigma}^r_{\gamma_0 l_0, \gamma_1 l_1}, \tag{25}$$

$$\bar{\sigma}^p_{\gamma_0 l_0, \gamma_1 l_1} = \frac{g(\Gamma_1)}{g(\gamma_0) Z^4 E_0} |T_{\Gamma_1 \Gamma_0}|^2 \pi a_0^2, \tag{25a}$$

$$\left.\begin{aligned} \bar{\sigma}^r_{\gamma_0 l_0, \gamma_1 l_1} &= \frac{g(\Gamma_1)}{2 g(\gamma_0) Z^4 E_0} \sum_\beta \tau^2_{\beta\Gamma_0}(\nu_\beta) \frac{\tau^2_{\beta\alpha}(\nu_\beta)}{\Sigma_\beta} [1 - \theta(E - \Delta E_{\beta\alpha})] \pi a_0^2, \\ \theta(x) &= 1, \quad x > 0, \quad \theta(x) = -1, \quad x < 0, \end{aligned}\right\} \tag{25b}$$

and Σ_β is defined in (21).

Thus, the averaged resonance cross section $\bar{\sigma}^r$ gives a contribution to the total cross section of the same order in the parameter Z^{-1} as $\bar{\sigma}^p$. Equation (25b) has a simple physical interpretation: The process of resonance excitation occurs through formation and decay of a doubly excited autoionized state β of the ion B_{Z-1} of the preceding multiplicity:

$$B_Z(\gamma_0) + e \to B^{**}_{Z-1}(\beta) \to B_Z^*(\gamma_1) + e. \tag{26}$$

The quantities $\tau^2_{\beta\alpha}$ which characterize the efficiency of capture into the level β obviously are proportional to the probability of autoionization decay $\Gamma_{\beta\alpha}$ of this level:

$$\Gamma_{\beta\alpha} = \frac{2}{\pi \nu_\beta^3 Z^2} |\tau_{\beta\alpha}|^2, \quad \Gamma_\beta = \sum_\alpha \Gamma_{\beta\alpha}. \tag{27}$$

The equations (25) were obtained on the usual assumption that the probabilities of radiative decay of the quasistationary states are $A_\beta \ll \Gamma_\beta$. The ratio A_β/Γ_β increases with increasing charge ($\sim Z^4$ for optically allowed transitions). In addition, A_β is practically independent of ν_β, since the main contribution to A_β is from the transition $n_\gamma \to n_{\gamma'}$ of the optical electron of the initial ion. Therefore with increasing Z the values of ν_β for which $\Gamma_\beta(\nu_\beta) \approx A_\beta$ decrease and, generally speaking, it is necessary to take into account the photon decay channel of the quasistationary states. Inclusion of this channel[7] leads to replacement in the denominator of Eq. (25b) of the probability Γ_β (which is proportional to Σ_α) by the total decay probability of the state β:

$$\Gamma_\beta \to \Gamma_\beta + A_\beta. \tag{28}$$

In this way we take into account the competing process of dielectron recombination

$$B_Z(\gamma_0) + e \to B^{**}_{Z-1}(\beta) \to B_{Z-1}(\beta') + \hbar\omega, \tag{29}$$

which is important for a number of applications (see, for example, ref. 12).

Using Eq. (28), we will rewrite expression (25) in the form

$$\bar{\sigma}_{\gamma_0 l_0, \gamma_1 l_1} = \sum_{\substack{l_0 l_1 \\ S_T L_T}} [\bar{\sigma}^p_{\gamma_0 l_0, \gamma_1 l_1} + \bar{\sigma}^r_{\gamma_0 l_0, \gamma_1 l_1}], \tag{30}$$

$$\left.\begin{aligned} \bar{\sigma}^r_{\gamma_0 l_0, \gamma_1 l_1} &= \frac{g(\Gamma_1)}{2 g(\gamma_0) Z^4 E_0} \sum_{\gamma' l'} \tau^2_{\gamma' l', \gamma_0 l_0} \frac{\tau^2_{\gamma' l', \gamma_1 l_1} [1 - \theta(E_0 - \Delta E_{\gamma' l'})]}{\Sigma_{\gamma' l'} + {}^1\!/_2 \pi Z^2 \nu_{\gamma'}^3 A_{\gamma' l'}}, \\ \Sigma_{\gamma' l'} &= \sum_{\gamma'' l''} \tau^2_{\gamma' l', \gamma'' l''}. \end{aligned}\right\} \tag{31}$$

Equations (30) and (31) have been written with use of L–S coupling, in which $\Gamma \equiv \gamma \cdot {}^1\!/_2 l \Gamma_T$; $\gamma \equiv (n_i l_i) n_\gamma l_\gamma LS$; $\Gamma_T \equiv S_T L_T$, where $n_i l_i$ are the quantum numbers of the core, $n_\gamma l_\gamma$ are the quantum numbers of the optical electron, L and S are the orbital and spin angular momenta of the initial ion; L_T and S_T are the orbital and spin angular momenta of the system ion + electron.

3. We will discuss as an example the cross sections for excitation of the transitions 2p – 3s and 2s – 3s in the lithium-like ion O VI calculated by means of Eqs. (30) and (31). The wave functions of the initial ion were calculated in terms of the semiempirical method of Vaĭnshteĭn.[13] It should be noted that the calculations are substantially simplified if we take into account that with increase of the principal quantum number n_γ of the closed channel, the quantities τ^2 approach the limiting value $n_\gamma^3 \tau^2 = \text{const}$, $n_\gamma \to \infty$. The question of the value of n_γ at which the asymptote is reached must be considered individually in each specific case; in the present case this approach occurs already for $n_\gamma \gg 5$.

The contribution of resonance scattering to excitation of a level with principal quantum number $n_{\gamma 1}$ is effective up to an incident-electron energy corresponding to the threshold of the open channel with $n_\gamma = n_{\gamma 1} + 1$ (see Figs. 1 and 2). In this energy interval the resonances converging to all closed levels with $n_\gamma > n_{\gamma 1}$ are important. In our case these levels are the levels with $n_\gamma = 3$ and all s levels with $n_\gamma \geq 4$, and for excitation of the 2p – 3s transition also all d levels. With increasing energy, resonance scattering leads to preferential excitation of the levels of new channels. The broken line in the figures shows the cross section σ^p for direct (potential) excitation. For the 2p – 3s transition the effect of resonance scattering determines the value of the cross section for incident-electron energies from the threshold 67.4 eV up to $E \approx 100$ eV. This situation is realized in cases in which there are effectively excited levels whose excitation thresholds exceed the threshold of the transition being studied. As an example we can point to the optic-

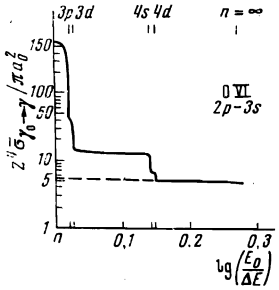

FIG. 1

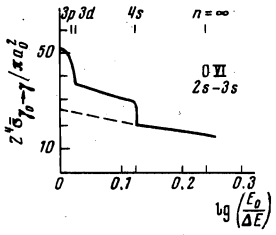

FIG. 2

FIG. 1. Cross section for excitation of the transition 2p–3s in the ion O VI. The broken line shows the cross section for potential scattering.

FIG. 2. Cross section for excitation of the 2s–3s transition in the ion O VI. The broken line shows the cross section for potential scattering.

ally forbidden transitions between fine-structure components in ground-state configurations of the type $2s^2 2p^k$, which present interest for astrophysical applications. In other cases the contribution of resonance scattering is not so large and, for example, for the 2s – 3s transition (Fig. 2) it is comparable with direct excitation. In the cross section for the intercombination transitions $1s(^1S) - 2p(^3P)$ in helium-like ions with charge $Z > 5$, resonance scattering is responsible for a correction $\lesssim 30\%$. We note also that the question of accuracy of the calculation of these cross sections is very urgent in study of the excitation mechanisms of x-ray spectra in the solar corona and in laboratory plasmas.

In connection with the above, special interest is presented by the direct experimental measurement of resonance scattering of electrons by multiply charged ions.

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