Energy dependence of the cross section for elastic scattering of slow electrons by positive ions at 180°

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The features of scattering of slow electrons by positive ions at 180° are discussed. The energy dependence of the cross section for scattering by the ions K^+, Na^+, Mg^{+2}, Yb^{+2}, V^{+5}, and Sc^{+3} is calculated. It is found that as a rule the cross sections at low energies are substantially greater than the Rutherford cross section. For the Na^+ ion a minimum in the cross section is observed at low energies.

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1. GENERAL RELATIONS

Let us consider the scattering of slow electrons by positive ions at an energy below the excitation threshold.

The amplitude for scattering by an ion with charge Z is

$$f(k,\theta)=f_{\text{Coul}}+\tilde{f}(k,\theta), \tag{1}$$

where the amplitude for scattering by the Coulomb field (in atomic units) is

$$f_{\text{Coul}}=\frac{Z\exp\{i[Zk^{-1}\ln(\sin^2(\theta/2))+2\eta_0]\}}{2k^2\sin^2(\theta/2)}, \qquad \eta_0=\arg\Gamma(1-iZ/k), \tag{2}$$

and $\tilde{f}(k,\theta)$ is an additional term due to the short-range part of the ion field.

The cross section, which is equal to $|f(k,\theta)|^2$, will contain a term

$$\sin[Zk^{-1}\ln\sin^2(\theta/2)],$$

which will lead to appearance of high-frequency oscillations in the energy dependence $\sigma(k,\theta)$ for a fixed angle θ. An exception is the case $\theta=\pi$, where $\ln(\sin^2(\theta/2))=0$. Here the high-frequency oscillations disappear and the cross section takes the form

$$\sigma(k,\pi)=\frac{Z^2}{4k^4}+\frac{Z}{k^3}\operatorname{Re}F(k)+\frac{1}{k^2}|F(k)|^2. \tag{3}$$

where F(k) denotes

$$F(k)=e^{2i\eta_0}\tilde{f}(k,\theta)/k. \tag{4}$$

As is well known, the amplitude $\tilde{f}(k,\theta)$ has the form[1]

$$\tilde{f}(k,\theta)=\frac{1}{2ik}\sum_l(2l+1)e^{2i\eta_l}(e^{2i\delta_l}-1)P_l(\cos\theta), \tag{5}$$

where $\eta_l=\arg\Gamma(l+1-iZ/k)$. Taking into account that $P_l(-1)=(-1)^l$ and introducing the designation

$$\varphi_l=2(\eta_l-\eta_0)+l\pi=2\sum_{n=1}^{l}\operatorname{arctg}\frac{mk}{Z}, \tag{6}$$

we obtain for F(k) the expression:

$$F(k)=\sum_l(2l+1)e^{i(\varphi_l+\delta_l)}\sin\delta_l. \tag{7}$$

The phase shifts δ_l in the presence of an attractive Coulomb field are finite for k = 0, and for small k they behave as

$$\delta_l(k)=\delta_l(0)+\delta_l'(0)\varkappa^2+O(\varkappa^4), \tag{8}$$

where $\varkappa=k/Z$.

In the region $\varkappa\ll 1$ the scattering cross section will be mainly Rutherford, i.e., in Eq. (3) the main role will be played by the first term. In the region $\varkappa\lesssim 1$ important contributions to the cross section will be made by the second and third terms.

The coefficients $\delta_l(0)$ and $\delta_l'(0)$ in Eq. (8) can be determined by extrapolation of the quantum defect $\mu_l(Z,n)$ for the ion of charge smaller by unity to the positive energy region.[2] For $n\gg 1$ we have

$$\mu_l(Z,n)=\mu_l(Z)+\mu_l'(Z)n^{-2}+O(n^{-4}). \tag{9}$$

Extension of Eq. (9) to the region of the continuum is obtained by the substitution

$$\mu_l(Z,n)\to\frac{1}{\pi}\delta_l(k), \quad n=\frac{Z}{ik}=\frac{1}{i\varkappa},$$

so that

$$\delta_l(k)=\pi\{\mu_l(Z)-\mu_l'(Z)\varkappa^2\}+O(\varkappa^4). \tag{10}$$

We note that addition of an integral multiple of π to the phase shift δ_l in Eq. (7) does not affect F(k); thus, for the calculations we actually need only the fractional part of the quantum defect. Therefore it may turn out that although $\mu_l\gg\mu_{l+1}$, the phase shift δ_{l+1} makes a more important contribution to F(k) than does δ_l. Consequently, in the sum (7) we cannot limit ourselves to one partial wave, but are forced to take into account several, the contribution of any of them possibly being considerably greater than the contribution of the s wave. Beginning with some l_0, all δ_l become appreciably less than π and with further increase of l rapidly fall off, so that in practice it is sufficient to take into account only $l\le l_0$.

2. SPECIFIC CALCULATIONS AND DISCUSSION

We calculated the cross sections for scattering of electrons by the ions Na^+, K^+, Mg^{+2}, Yb^{+2}, Sc^{+3}, and V^{+5}. For the last four ions we used the quantum-defect method described above, which gives the possibility of obtaining results in the energy region considered without assuming a specific form of the short-range potential. For the ions Na^+ and K^+ the quantum-defect method was used only for $k\ll 1$. For higher energies we substituted in Eq. (3) directly the values of the phase shifts δ_l found in the Hartree-Fock approximation.[1)] The data for the coefficients $\mu_l(Z,n)$ and $\mu_l'(Z,n)$ were taken from refs. 3–7.

A characteristic feature of all of the cross sections obtained is the fact that, beginning with some value of κ equal to several tens of atomic units, they are much greater than the Coulomb cross section.

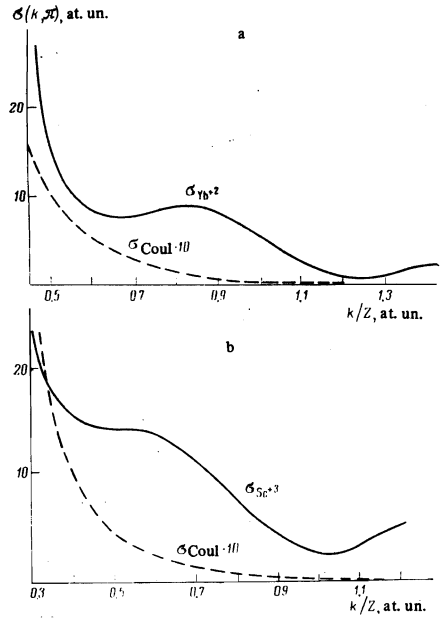

FIG. 1. Cross section for scattering by the ion Yb^{+2} (a) and by Sc^{+3} (b). The dashed curve is the cross section for scattering by a Coulomb field, $\sigma_{Coul} = Z^2/4k^4$, increased by a factor of ten.

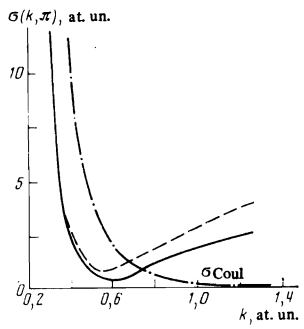

FIG. 2. Cross section for scattering of electrons by Na^+ ions. The solid curve is for calculation of the first three phase shifts δ_l in the Hartree-Fock approximation and determination of δ_3 and δ_4 by the quantum-defect method; the dashed curve is for calculation of all phase shifts $\delta_l (l \geqslant 4)$ taken into account in the calculation by the quantum-defect method; the dot-dash curve is the cross section for scattering by the Coulomb field, $\sigma_{Coul} = Z^2/4k^4$.

In Fig. 1 we have shown the change of the scattering cross sections with increase of κ for Yb^{+2} and Sc^{+3}. The discussion has been limited to values $\kappa \lesssim 1$, i.e., to that energy region where we are still far from the first excitation threshold. The oscillations are produced by the change in the interference amplitude F(k), which for the given energy values makes the main contribution to the cross section $\sigma(k,\pi)$. For the ions K^+, Mg^{+2}, and V^{+5}, oscillations in the cross section were also obtained, but for energies lying either beyond the excitation threshold (K^+) or in the region where the quantum-defect approximation is inapplicable (Mg^{+2}, V^{+5}).

For $\kappa \ll 1$ the cross section $\sigma(k,\pi)$ can be expanded in series in κ. Then

$$\sigma = Z^{-2}(^1/_4\kappa^{-4} + A\kappa^{-3} + B\kappa^{-2}),$$

where A and B are constants which do not depend on energy. It is evident that for $A = \mathrm{Re}\, F(0) < 0$ it is possible for the differential cross section σ to have a minimum and to become smaller than the Coulomb cross section. This phenomenon is similar to the Ramsauer minimum which arises in the total cross section for scattering of electrons by atoms of the noble gases and which is due to the action of the long-range potential. The cause of the effect discussed in the present work is the Coulomb Interaction. However, while the Ramsauer effect in a neutral atom is explained by the vanishing of the partial s wave, in the present case the minimum appears as a result of the interference of waves with several different values of l. This effect can be observed also for not too small values of κ, but in this case it is not of interest since the cross section as a whole is small.

A minimum of the Ramsauer type was found in calculation of the scattering by Na^+ ($A = -0.61$). The cross section for backward scattering by the Na^+ ion is shown in Fig. 2 as a function of energy.

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[1)] In calculation of the phase shifts in the Hartree-Fock approximation we used programs written by N. A. Cherepkov and L. V. Chernysheva.

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