THEORY OF ANOMALIES IN THE DIFFERENTIAL SCATTERING CROSS SECTIONS FOR HIGH-ENERGY ATOMS IN THE PRESENCE OF AN INELASTIC PROCESS

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The form of the differential scattering cross sections (elastic and inelastic) for high-energy atoms in the presence of an inelastic process involving quasi-intersection of terms is investigated. It is shown the oscillations in the inelastic cross section at angles greater than the threshold value τ_{th} are the result of interference of contributions from two trajectories. From the experimental phase of the oscillations,[1,2] one can find the parameters of the scattering functions contributing to the process, and some of the potential parameters. It is shown that in a certain range of angles ($\tau_{th}^{e} < \tau < \tau_0$) close to the angle τ_{th}^{e} at which the anomalies set in in the elastic cross section, the latter is the result of interference of contributions from three trajectories (or three branches of the scattering function); at larger values ($\tau > \tau_0$), two scattering trajectories contribute. Quasi-classical expressions are obtained which are replaced by quantum expressions in the vicinity of the threshold angles τ_{th}, τ_{th}^{e} and of the angle τ_0 corresponding to the term intersection radius R_0. The calculated form of the elastic cross section, in which a certain approximation is used for the scattering functions, agrees qualitatively with experiment and enables us to formulate a prescription for determining the term intersection radius R_0 from experimental curves for the elastic cross section.

THE intensive measurements of differential scattering cross sections recently carried out have made it possible to reveal a number of fine details that were previously inaccessible. Thus, differential cross sections are presented in [1,2] for elastic and inelastic scattering of He^+ by Ne (Ar) and these indicate unambiguously that the inelastic process (excitation of Ne into a $2p^5 3s$ state) is due to intersection of the ground and excited terms. The cross sections for these processes (as for many others not mentioned here) display characteristic "Stueckelberg" oscillations, associated with the fact that different trajectories can make a contribution to the scattering (elastic and inelastic) at a given angle (since a transition is possible for both forward and backward radial motion in the term-intersection region).

To extract the potential parameters from the details of these oscillations, we need a theory of such oscillations near the threshold of the inelastic channel. In [3-6], different variants are given of a quasi-classical description of the phenomenon, in which the amplitudes and phases of two interfering contributions to the cross section are described by classical actions along the corresponding trajectories. Close to the threshold, however, such a simple description is inapplicable, and a more detailed quasi-classical analysis (and at certain angles a quantum analysis) is necessary. For an inelastic process close to the threshold, such an analysis was performed in [7].

In the present work a theory is developed of the anomalies in the elastic scattering near the threshold of an inelastic process due to quasi-intersection of terms. We consider the case of high energies, when the analysis of the cross sections becomes comparatively simple. For the sake of generality, in addition to deriving new results for the elastic scattering we also repeat the derivation of the expression for the inelastic cross section, in a form which is different from [7] and more general and intuitive. We apply the theory to discuss the experimental data of [1,2] for the system He^+–Ne.

As always, at high energies we shall use reduced variables for the angles and cross sections

$$\tau = E\theta, \quad \rho_{ij}(\tau, E) = \theta \sin\theta \cdot \sigma_{ij}(\theta, E), \tag{1}$$

where E is the energy of relative motion of the colliding pair, and θ and $\sigma_{ij}(\theta, E)$ are the scattering angle and differential cross section for scattering with a transition from state i to state j.

We consider the simplest, but often encountered (cf., e.g., [8]) situation, when the inelastic process can be described with a basis set of only two adiabatic electron states, the terms (potential functions) of which have a quasi-intersection in the vicinity of the point R_0. In such a case, from this adiabatic basis set it is easy to construct a "diabatic" basis set[9] $\{\varphi_1(R, r_i)\varphi_2(R, r_i)\}$, in which the Schrödinger equation for the wavefunction

$$\psi(\mathbf{R}, \mathbf{r}_i) = \chi_1(\mathbf{R})\varphi_1(R, \mathbf{r}_i) + \chi_2(\mathbf{R})\varphi_2(R, \mathbf{r}_i) \tag{2}$$

is described only by a potential matrix, without a differential non-adiabatic coupling:

$$\frac{1}{2m}\Delta_R\begin{pmatrix}\chi_1(\mathbf{R})\\ \chi_2(\mathbf{R})\end{pmatrix} = \begin{pmatrix}V_1(\mathbf{R}) & V_{12}(\mathbf{R})\\ V_{21}(\mathbf{R}) & V_2(\mathbf{R})\end{pmatrix}\begin{pmatrix}\chi_1(\mathbf{R})\\ \chi_2(\mathbf{R})\end{pmatrix}. \tag{3}$$

Here and below, $\hbar = 1$, and m is the reduced mass of the pair of atoms. The terms $V_1(R)$ and $V_2(R)$ of the "zeroth" (not including V_{12}) approximation intersect at the point R_0 and at large distances correspond to the excitation energy $\Delta E = V_2(\infty) - V_1(\infty)$.

In the well-known high-energy approximation (or the impact-parameter approximation,[10, 11, 18] the nuclear wavefunctions $\chi_j(R)$ have the form of modulated plane waves

$$\chi_j(R)=e^{ikz}c_j(b,z)\exp\left\{-i\frac{1}{u}\int\limits_{-\infty}V_j(R')dz'\right\},$$

$R'=\sqrt{b^2+z'^2}$, with amplitudes c_j satisfying the first-order equations:

$$i\frac{dc_j}{dz}=\frac{1}{u}V_{jk}\exp\left\{-\frac{i}{u}\int\limits_{-\infty}^{z}(V_j-V_k)dz'\right\}c_k;\ j\neq k,\ j,k=1.2 \quad (4)$$

and the appropriate boundary conditions: $c_j(z=-\infty)=\delta_{jj_0}$. Here, b is the impact parameter, $k=\sqrt{2mE}$ is the momentum and $u=\sqrt{2m/E}$ is the relative velocity.[1)] The differential scattering amplitudes $f_{jk}(\theta)$ are expressed in terms of the transition amplitudes $c_j(b, z=+\infty)$ in the usual way,[8, 12] replacing the sum over the angular momenta l by an integral over the impact parameter $b=\hbar(1+\frac{1}{2})/mu$.

For elastic scattering with each of the unperturbed potentials $V_1(R)$ and $V_2(R)$, the high-energy approximation leads to the following equations for the corresponding scattering functions $b_1^0(\tau)$ and $b_2^0(\tau)$ connecting the scattering angle with the impact parameter:

$$-b\left[\int\limits_{-\infty}^{\infty}\frac{1}{R}\frac{dV_j(R)}{dR}dz\right]\Bigg|_{b=b_j^0(\tau)}=\tau;\quad R^2=b^2+z^2. \quad (5)$$

Equation (5) is the well-known[13] formula for classical scattering through small angles and reflects the well-known correspondence principle (cf., e.g., [1]) which states that at high energies the reduced cross section $\rho_j^0(\tau)=\frac{1}{2}db_j^2(\tau)/d\ln\tau$ depends only on one combination $\tau=E\theta$ of the two variables E and θ.

Figure 1 shows the form of $b^0_{1(2)}(\tau)$ (more, correctly, the inverse functions $\tau^0_{1(2)}(b)$) for the case when $V_1(R)$ is a purely repulsive potential and $V_2(R)$ is weakly attractive at large distances. The function $b_1^0(\tau)$ for unperturbed elastic scattering is monotonic, so that small angles τ correspond to large b. On the basis of this, it was assumed[1, 2] that the angle τ characterizing the beginning (from the side of small τ) of the oscillations in the elastic channel corresponds to the maximum impact parameter for which the trajectory

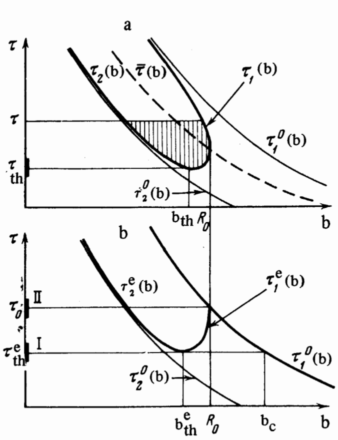

FIG. 1. Form of the scattering function. The functions $\tau_1^0(b)$, $\tau_2^0(b)$ and $\bar\tau(b)$ correspond to scattering in the potentials $V_1(R)$, $V_2(R)$ and $\bar V=\frac{1}{2}(V_1+V_2)$. (a) The scattering functions $\tau_1(b)$ and $\tau_2(b)$ for the inelastic process; (b) the scattering functions $\tau_1^e(b)$, $\tau_2^e(b)$ and $\tau_1^0(b)$ for the elastic process. The marked parts of the τ-axis indicate the regions of violation of the quasi-classical description.

touches the region of intersection; this value of the impact parameter consequently coincides with the radius R_0 of the intersection of the terms. However, as we shall see below, this assumption is not correct, since the scattering functions for atoms under the influence of a combination of two potentials $V_1(R)$ and $V_2(R)$ do not possess the monotonic character that $b_1^0(\tau)$ has.

At energies E greater than the value E_{max} at which the inelastic scattering reaches its maximum, the motion of the system derives mainly[8, 9] from the diabatic terms V_1 and V_2, so that we can use perturbation theory in the interaction V_{12} between the states φ_1 and φ_2 to calculate the transition amplitudes from (4). Then the reduced cross sections $\rho_{11}(\tau)$ and $\rho_{12}(\tau)$ for elastic and inelastic scattering, correct to terms of second order in V_{12}, are written in the form

$$\rho_{11}=\frac{\tau}{2\pi}\left|\int\limits_0^\infty\sqrt{\frac{2b}{u}}db\left\{e^{iS_1^0(b,\tau)}-\int\limits_{-\infty}^{\infty}\frac{dz}{u}V_{12}(R)\int\limits_{-\infty}^{z}\frac{d\tilde z}{u}V_{21}(\tilde R)e^{iS^e(b,z,\tilde z,\tau)}\right\}\right|^2, \quad (6)$$

$$\rho_{12}=\frac{\tau}{2\pi}\left|\int\limits_0^\infty\sqrt{\frac{2b}{u}}db\int\limits_{-\infty}^{\infty}\frac{dz}{u}V_{12}(R)e^{iS(b,z,\tau)}\right|^2;$$
$$R=(b^2+z^2)^{1/2},\quad \tilde R=(b^2+\tilde z^2)^{1/2}. \quad (7)$$

Here the action[2)]

$$S_1^0(b,\tau)=\frac{1}{u}\left\{-\int\limits_{-\infty}^{\infty}V_1(R)dz-2b\tau\right\} \quad (8)$$

corresponds to the unperturbed motion through the term $V_1(R)$. The action $S^e(b, z, \tilde z, \tau)$ corresponds to elastic scattering with transitions at the points z and $\tilde z$:

$$S^e(b,z,\tilde z,\tau)=\frac{1}{u}\left\{-\int\limits_{-\infty}^{\infty}V_1(R')dz'+\int\limits_{\tilde z}^{z}\Delta V(R')dz'-2b\tau\right\}, \quad (9)$$
$$\Delta V=V_1-V_2,\quad R'=(b^2+z'^2)^{1/2}.$$

Finally, the action $S(b, z, \tau)$ corresponding to the inelastic process is equal to

$$S(b,z,\tau)=\frac{1}{u}\left\{2\int\limits_0^\infty\frac{1}{R'}\frac{d\bar V(R')}{dR'}(z')^2dz'-\int\limits_0^z\Delta V(R')dz'-2b\tau\right\}, \quad (10)$$

where $\bar V=\frac{1}{2}(V_1+V_2)$ is the average potential.

In view of the quasi-classical nature of the atomic motion (the exponentials e^{iS} oscillate rapidly), the integrals in (6) and (7) can be investigated by the stationary phase (s.p.) method.

1. We begin with the simpler inelastic scattering. The stationary phase (s.p.) conditions in each of the integration variables b and z in (7) uniquely determine the scattering-function branches $b_\nu(\tau)$ and $z_\nu(\tau)$ contributing to the inelastic process. In fact, the first of these conditions has the form

$$\partial S(b,z,\tau)/\partial z=\Delta V(b,z)=0, \quad (11)$$

which means that the (s.p.) point (z_ν, b_ν) lies on the radius of intersection of the terms:

$$z_\nu(\tau)=\pm\sqrt{R_0^2-b_\nu^2(\tau)}. \quad (12)$$

When (12) is taken into account, the s.p. condition in b leads to an equation for the branches $b_\nu(\tau)$:

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1) At high energies $E\gg\Delta E$, the difference between the velocities for each term can be neglected.

2) The sign of the term $\pm 2b\tau/u=\pm(1+\frac{1}{2})\theta$ chosen in (8)–(10) corresponds to repulsion [8, 12].

$$b\left[\int_0^\infty \frac{1}{R}\frac{d\overline{V}(R)}{dR}dz + \int_0^{\pm\sqrt{R_0^2-b^2}} \frac{1}{R}\frac{d(\Delta V)}{dR}dz\right]\Bigg|_{b=b_\nu(\tau)} = 2\tau. \quad (13)$$

The characteristic form, resulting from (13), of the two branches ($\nu = 1, 2$) of the scattering function $\tau(b)$ that contribute to the inelastic process is depicted in Fig. 1a. We shall clarify it. A comparison of (13) and (5) shows that for large τ, when the scattering is determined mainly by the behavior of the potentials at small distances $R < R_0$, the branches $\tau_1(b)$ and $\tau_2(b)$ merge respectively into the functions $\tau_1^0(b)$ and $\tau_2^0(b)$ for unperturbed scattering in the potentials $V_1(R)$ and $V_2(R)$ (see Fig. 1a). Further, on decrease of τ, the function $\tau_1(b)$ touches the straight line $b = R_0$ at the point $b = R_0$, $\tau = \overline{\tau}_0 = \overline{\tau}(R_0)$, where $\overline{\tau}(b)$, which is the scattering function in the average potential $\overline{V}(R)$, is depicted in Fig. 1a by a dashed line; $z_1(\tau)$ changes sign at the point $\tau = \overline{\tau}_0$. In fact, differentiating Eq. (13), in which we can regard b as the independent variable with $\tau = \tau_1(b)$, with respect to b, we obtain the following expansion of $\tau_1(b)$ in the vicinity of the point $(\overline{\tau}_0, R_0)$:

$$R_0 - b_1(\tau) = \frac{2}{R_0(\Delta F)^2}(\tau - \overline{\tau}_0)^2 + \ldots, \quad (14)$$

where $\Delta F = F_1 - F_2$ is the difference in the slopes $F_j = dV_j(R)/dR|_{R_0}$ of the terms at the point of intersection.

Finally, at a certain threshold value of the angle τ_{th} determined from the equation $d\tau_\nu(b)/db|_{b_{th}} = 0$, the branches $b_1(\tau)$ and $b_2(\tau)$ run together, being inverse functions of a single function $\tau(b)$, and in the vicinity of the point $(\tau_{th}, b_{th} = b_1(\tau_{th}) = b_2(\tau_{th}))$ have the form

$$b_\nu(\tau) = \pm\sqrt{\frac{2(\tau - \tau_{th})}{\varkappa}} + \ldots \quad (15)$$

Here, $\kappa = d^2\tau_\nu(b)/db^2|_{b_{th}}$.

From the described form of the functions $\tau_\nu(b)$ ($\nu = 1, 2$) (Fig. 1a), it is clear that for angles less than the threshold angle $\tau < \tau_{th}$ inelastic scattering is absent, while for $\tau > \tau_{th}$ the inelastic scattering is the result of the interference of the two contributions from the two branches $b_1(\tau)$ and $b_2(\tau)$ of the scattering function. A calculation of these contributions by the s.p. method gives the following expression for the inelastic cross section:

$$\rho_{12}(\tau) = |\sqrt{\rho_1(\tau)p_1}e^{iS_1(\tau)} - \sqrt{\rho_2(\tau)p_2}e^{iS_2(\tau)-i\pi/2}|^2. \quad (16)$$

Here,

$$\rho_\nu(\tau) = \tau b_\nu(\tau)db_\nu/d\tau$$

are the reduced cross sections corresponding to the functions $b_\nu(\tau)$; $p_\nu = p(b_\nu(\tau))$ is the Landau–Zener transition probability between the terms (in lowest order in V_{12}), which depends on the radial velocity u_R at the point of intersection:

$$p(b) = \frac{2\pi V_{12}^2}{u_R(b)\hbar\Delta F}; \quad u_R(b) = u\frac{\sqrt{R_0^2 - b^2}}{R_0}. \quad (17)$$

The phases $S_\nu(\tau)$ ($\nu = 1, 2$) in (16) are the values of the action (10) at the s.p. points: $S_\nu = S(b_\nu(\tau), z_\nu(\tau), \tau)$. The small phases 0 and $\pi/2$ for each contribution in (16) are determined by the signs of the eigenvalues of the matrix of the second derivatives of the action; this matrix is

$$\hat{D}^{(\nu)}_{b,z} = \begin{pmatrix} \frac{\partial^2 S}{\partial z^2} & \frac{\partial^2 S}{\partial z\partial b} \\ \frac{\partial^2 S}{\partial b\partial z} & \frac{\partial^2 S}{\partial b^2} \end{pmatrix}\Bigg|_{b_\nu, z_\nu} = \begin{pmatrix} -\frac{z_\nu\Delta F}{uR_0} & -\frac{b_\nu\Delta F}{uR_0} \\ -\frac{b_\nu\Delta F}{uR_0} & \frac{1}{u}\left[2\frac{d\tau_\nu}{db} - \frac{b_\nu^2\Delta F}{R_0 z_\nu}\right] \end{pmatrix}.$$

The difference in the actions $\Delta S = S_1(\tau) - S_2(\tau)$, which, according to (16), controls the interference structure of the inelastic cross section, can easily be expressed in terms of the characteristics of the scattering functions $b_\nu(\tau)$:

$$\Delta S(\tau) = -\frac{2}{u}\int_{\tau_{th}}^{\tau} \Delta b(\tau)d\tau, \quad \Delta b(\tau) = b_1(\tau) - b_2(\tau). \quad (18)$$

Thus, the phase of the oscillations in the inelastic cross section is uniquely determined by the area of the shaded portion in Fig. 1a.

Quasi-classical expressions of the type (16) for the cross section ρ_{ij} were adduced in [3-6]. However, at angles close to the threshold angle, the expression (16) diverges and becomes inapplicable. The reason for this is that the s.p. method is inapplicable in the vicinity of the point τ_{th}. The s.p. method assumes a quadratic form for the action in the exponential in (7) in the vicinity of the s.p. point. This requires, at least, that the determinant of this quadratic form, defined by the expression:

$$|\mathrm{Det}\,\hat{D}_{bz}| = \left|\frac{\partial^2 S}{\partial b^2}\frac{\partial^2 S}{\partial z^2} - \left(\frac{\partial^2 S}{\partial b\partial z}\right)^2\right|_{b_\nu z_\nu} = -\frac{z_\nu\Delta F}{uR_0}\frac{d\tau_\nu(b)}{db}\Bigg|_{b_\nu}. \quad (19)$$

be non-zero. But, by virtue of the definition of the threshold point $(d\tau_\nu/db|_{\tau_{th}} = 0)$, we have $\mathrm{Det}\, D_{bz}|_{\tau_{th}} = 0$. This means that to calculate the integral in (7) in the vicinity of the point τ_{th}, the quadratic expansion of the action $S(b, z, \tau)$ must be supplemented by the necessary terms of third order in $\Delta b = b - b_{th}$ and $\Delta z = z - z_{th}$ ($z_{th} = \sqrt{R_0^2 - b_{th}^2}$); this leads to the following form for the action in the vicinity of the point z_{th}, b_{th}, τ_{th}:

$$S = -\frac{2b_{th}}{u}\Delta\tau + \left(-\frac{2\Delta\tau}{u}\frac{b_{th}}{R_0}\xi - \frac{R_0\Delta F}{uz_{th}}\xi^2\right) + \left[\frac{2}{u}\Delta\tau\frac{z_{th}}{R_0}\eta - \frac{\varkappa}{3u}\left(\frac{z_{th}}{R_0}\eta\right)^3\right],$$

$$\xi = \frac{z_{th}}{R_0}\Delta z + \frac{b_{th}}{R_0}\Delta b, \quad \eta = \frac{b_{th}}{R_0}\Delta z - \frac{z_{th}}{R_0}\Delta b.$$

The calculation of (7) with the above action gives for the inelastic cross section close to the threshold an expression analogous to that encountered in the description of the rainbow phenomenon in potential scattering:[13]

$$\rho_{12}(\tau) \approx 4p(b_{th})\frac{\tau b_{th}}{u}\left(\frac{\varkappa}{u}\right)^{-2/3}\Phi^2\left(-\frac{2\Delta\tau}{u}\left(\frac{\varkappa}{u}\right)^{-1/3}\right); \quad \varkappa = \frac{d^2\tau}{db^2}\Bigg|_{b_{th}}. \quad (20)$$

Here, $\Phi(x)$ is the Airy function (cf. [7]) and $p(b)$ is the probability defined by formula (17). The expression (20) gives exponential attenuation of the cross section for $\tau < \tau_{th}$ and goes over to the quasi-classical oscillations (16), (18) for $\tau > \tau_{th}$.

The formula (20) for the inelastic cross section was obtained in slightly different variables in [7], in which it was shown on the basis of experimental data for the system He^+–Ne from [2] that the periods in τ of the first (above the threshold) oscillations of $\rho_{12}(\tau E)$ are, as also follows from (20), linear functions of $E^{1/3}$ (in contrast to the dependence $E^{1/2}$ which follows from the quasi-classical formula (16)). On the basis of these dependences, and also of the energy dependence of the amplitude of the first peak in the cross section, the parameters characterizing the system of the intersecting terms responsible for the excitation of Ne have been determined.[7] Written in the notation of the present paper, these parameters are equal to

$$\tau_{th} \approx 930\ \text{eV-deg};\ \varkappa = 14.0\ \text{at.un.};\ \frac{V_{12}{}^2 b_{th}}{z_{th} \Delta F} \approx (1.5-1.8)10^{-4}\ \text{at. un.} \tag{21}$$

These parameters were obtained from the characteristics of the cross section ρ_{12} within the first oscillation period from the threshold. But it follows from (16) and (18) that the experimental phase of the oscillations for larger τ can be used to extract information about the dependence $\Delta b(\tau)$ not only close to the threshold. In fact, at large τ (starting from the second period of $\rho_{12}(\tau)$), the experimental phase $2\pi N(\tau, E)$ of the cross-section oscillations, where $N = 1, 2, \ldots$ at the peaks in the cross section and $N = 3/2, 5/2, \ldots$ at the minima, determines the energy-independent integral:

$$I(\tau) = \frac{1}{\pi u_0} \int_{\tau_{th}}^{\tau} \Delta b(\tau)\, d\tau = E^{1/2}\left[N(\tau E) - \frac{3}{4} \right], \quad N \geqslant 2, \tag{22}$$

where u_0 is the velocity corresponding to an energy of 1 eV, so that $u(E) = u_0\sqrt{E}$, where E is in eV. At the points $\tau_1, \tau_{3/2}, \tau_2$ characterizing the position of the first peak in the cross section ρ_{12}, it follows from the quantum formulas that the function $I(\tau)$ has the form

$$I(\tau_N) = \frac{2}{3\pi} (x_N)^{3/2} E^{1/2}, \quad N \leqslant 2, \tag{23}$$

where x_N is the value of the argument of the Airy function $\Phi(x)$ corresponding to the extrema ($N = 1, 2, \ldots$)

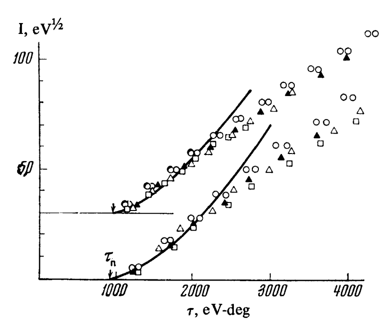

FIG. 2. The function $I(\tau)$, which characterizes the phase of the oscillations in the inelastic cross section, constructed from the definitions (25) and (26) on the basis of experimental data from [2] for τ_N in the system He^+–Ne. The points on the lower curve correspond to the following energies in eV: ○–500, ▲–417, □–376, △–333; on the upper curve (which is displaced along the vertical by 30 eV$^{1/2}$): ▲–292, ○–250, △–167, □–125. The solid curve is the theoretical dependence of $I(\tau)$ near the threshold.

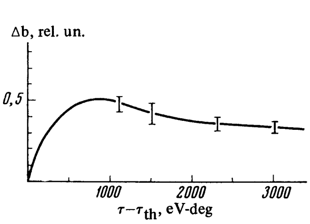

FIG. 3. The experimentally established relative position $\Delta b(\tau) = b_1(\tau) - b_2(\tau)$ of the two scattering-function branches contributing to the inelastic process.

or the zeros ($N = 3/2, 5/2, \ldots$) of $\Phi(x)$. For values of N starting from $N = 2$, we have $x_N = [(3\pi/2)(N - 3/4)]^{2/3}$, so that the definitions (22) and (23) of the function $I(\tau)$ coincide. In Fig. 2, the points show the dependence $I(\tau)$ constructed on the basis of formulas (22) and (23) and the experimental data for τ_N at different energies from [2]. The solid curve depicts the theoretical behavior of $I(\tau)$ near the threshold

$$I(\tau) = \frac{8}{3} \frac{1}{u_0} \sqrt{\frac{2}{\varkappa}} (\tau - \tau_{th})^{3/2} \tag{24}$$

with the parameters τ_{th} and κ predicted previously[7] (cf. (21)).

Differentiation with respect to τ of the average experimental curve makes it possible to obtain the dependence $\Delta b(\tau)$ depicted in Fig. 3. However, it is not possible to make a more accurate estimate of ΔF than that given in [7] $\Delta F = 20 - 60$ eV/a.u., since we know only the relative Δb, and not the absolute positions of the two branches $b_1(\tau)$ and $b_2(\tau)$.

2. We turn to the more complicated analysis of the elastic scattering, the cross section (6) of which can be conveniently rewritten in the form (also exact to terms $\sim V_{12}^2$)

$$\rho_{11}(\tau) = \rho_1{}^0(\tau) + \Delta\rho(\tau E);$$

$$\Delta\rho = -2\sqrt{\frac{\tau \rho_1{}^0(\tau)}{\pi u}} \operatorname{Re}\left\{ \exp\left[-iS_1{}^0(b_1{}^0(\tau), \tau) + \frac{i\pi}{4} \right] \int_0^\infty db \sqrt{b} \int_{-\infty}^{\infty} \frac{dz}{u} \int_{-\infty}^{z} \frac{d\tilde{z}}{u} \times V_{12}(R) V_{21}(\tilde{R}) \exp[iS^e(b, z, \tilde{z}, \tau)] \right\}, \tag{25}$$

where $\rho_1^0(\tau) = \tau b_1^0(\tau) db_1^0/d\tau$ is the cross section for unperturbed scattering by the first term and S_1^0 and S^e are defined by the formulas (8)–(9). The phase $\pi/4$ in (25) has appeared as a result of calculating the unperturbed scattering amplitude by the s.p. method and allowing for the fact that

$$\partial^2 S_1{}^0 / \partial b^2 = d\tau_1{}^0 / db < 0.$$

We shall calculate the integrals in (25) by the s.p. method (where this is applicable). The s.p. conditions in the variables z and $\tilde{z}$ for the exponential in the integrand in (25): $\partial S^e/\partial z = \partial S^e/\partial \tilde{z} = 0$, where S^e is defined by (9), can be written in the form $\Delta V(R) = \Delta V(\tilde{R}) = 0$, which means that the points $(b, \tilde{z})$ and (b, z) lie on the intersection radius. With allowance for the fact that $z \geq \tilde{z}$, this leads to three possible for the s.p. points in z and $\tilde{z}$:

$$\begin{aligned} &\text{a)}\ z = \tilde{z} = +\sqrt{R_0{}^2 - b^2}, \\ &\text{b)}\ z = \tilde{z} = -\sqrt{R_0{}^2 - b^2}, \\ &\text{c)}\ z = -\tilde{z} = +\sqrt{R_0{}^2 - b^2}, \end{aligned} \tag{26}$$

the realization of which will depend on the angle τ. Imposing then an additional s.p. condition in the variable b ($\partial S^e/\partial b = 0$), we obtain, in conjunction with (26), equations for the branches $\tau_\nu^e(b)$ of the scattering function that contribute to $\Delta\rho$, for each of the possibilities a), b) and c) in (26):

$$\text{a), b)} \quad -b\left[\int_{-\infty}^{\infty} \frac{1}{R} \frac{dV_1}{dR} dz \right] = \tau_1{}^0(b), \tag{27}$$

$$\text{c)} \quad -b\left[\int_{-\infty}^{\infty} \frac{1}{R} \frac{dV_1}{dR} dz - 2 \int_0^{+\sqrt{R_0^2 - b^2}} \frac{1}{R} \frac{d\Delta V(R)}{dR} dz \right] = \tau^e(b).$$

According to (5), the first Eq. (27) determines the function $\tau_1^0(b)$ for unperturbed scattering by the first term. In conjunction with conditions (26a, b), this means that there will be a contribution to $\Delta\rho$ from this branch only when $\tau > \tau_0 = \tau_1^0(R_0)$. In fact, for smaller $\tau (\tau < \tau_0)$, we have (cf. Fig. 2a): $b_1^0(\tau) > R_0$, so that the corresponding z and $\tilde{z}$ in (26a, b) turn out to be imaginary. The combined contribution (from (a) and (b)) to $\Delta\rho$ from the branch $\tau_1^0(b)$ when $\tau > \tau_0$ can be easily calculated and is equal to the second term in the final formula (30).

We shall now investigate the scattering-function branches $\tau_\nu^e(b)$ satisfying Eq. (27), which also contribute to the elastic scattering. The investigation of (27c) is completely analogous to that of Eq. (13) and gives the following characteristic form of the two branches $b_\nu^e(\tau)$, $\nu = 1, 2$ (which differ from the $b_\nu(\tau)$ for the inelastic process) (Fig. 1b). At large τ, we have only one branch $b_2^e(\tau)$, which merges with $b_2^0(\tau)$, the function for unperturbed scattering by the term $V_2(R)$. In fact, scattering through large angles is due mainly to the influence of strong repulsion at distances $R < R_0$, at which the effective potential in Eq. (27c) is the potential of the second term: $V_1 - \Delta V = V_2(R)$. On decrease of the angle from $\tau = \tau_0 = \tau_1^0(R)$, in addition to the branch $b_2^e(\tau)$ there appears another branch $b_1^e(\tau)$, which also satisfies (27c). Its form in the vicinity of τ_0 is completely determined by the difference between the slopes of the terms at the intersection point (compare with (14)):

$$b_1^e(\tau)\,|_{\tau\sim\tau_0} = R_0 - \frac{1}{2R_0(\Delta F)^2}(\tau-\tau_0)^2 + \dots. \quad (28)$$

Finally, at a certain threshold point τ_{th}^e (differing from τ_{th}, the threshold in the inelastic channel), the two branches $b_1^e(\tau)$ and $b_2^e(\tau)$ merge, being two branches of a single inverse function $\tau^e(b)$ satisfying Eq. (27c) (in Fig. 1b, the different parts of the function $\tau^e(b)$ are denoted by the subscripts 1 and 2); the threshold τ_{th}^e and the form of $b_\nu^e(\tau)$ close to τ_{th}^e are determined from the equations:

$$\left.\frac{d\tau^e(b)}{db}\right|_{b_{th}^e} = 0; \quad b_\nu{}^e(\tau)\Big|_{\tau\sim\tau_{th}^e} = b_{th}{}^e \pm \sqrt{\frac{2}{\varkappa^e}(\tau-\tau_{th}{}^y)}. \quad (29)$$

Here, $\kappa^e = d^2\tau^e/db^2|_{\tau_{th}^e}$. The calculation of the contributions to $\Delta\rho$ corresponding to the branches $b_1^e(\tau)$ and $b_2^e(\tau)$ is performed by the usual s.p. method. As regards the contributions from the two regions $b \sim b_1^0(\tau)$, $z \approx \tilde{z} \approx \pm\sqrt{R_0^2 - (b_1^0)^2}$, their sum reduces to a Gaussian integral when the symmetry of the potential $(V_i(b, z) = V_i(b, -z))$ is taken into account.

The final expressions for $\Delta\rho(\tau)$ in the different regions of variation of τ have the form:

$$\Delta\rho(\tau) = 2\sqrt{\rho_1{}^0(\tau)\rho_2{}^e(\tau)}\,p(b_2{}^e(\tau))\cos[S_2{}^e - S_1{}^0 + \pi/2] - 2\rho_1{}^0(\tau) \times p(b_1{}^0(\tau)),\ \tau > \tau_0; \quad (30)$$

$$\Delta\rho(\tau) = 2\sqrt{\rho_1{}^0(\tau)\rho_2{}^e(\tau)}\,p(b_2{}^e(\tau))\cos[S_2{}^e(\tau) - S_1{}^0(\tau) + \pi/2] - 2\sqrt{\rho_1{}^0(\tau)\rho_1{}^e(\tau)}\,p(b_1{}^e)\cos[S_1{}^e(\tau) - S_1{}^0(\tau)],\quad \tau_{th}^e < \tau < \tau_0 \quad (31)$$

Here, $\rho_\nu^e(\tau) = \tau b_\nu^e(\tau) db_\nu^e/d\tau$; the probability p(b) is defined by formula (17), and $S_\nu^e(\tau) = S^e(b_\nu(\tau), z_\nu, \tilde{z}_\nu, \tau)$ and $z_\nu = -\tilde{z}_\nu = \sqrt{R_0^2 - b_\nu^2}$. The relative values of the actions in (30) and (31) can be expressed, similarly to (18), as follows in terms of the characteristics of the scattering functions:

$$S_1{}^e(\tau) - S_1{}^0(\tau) = \frac{2}{u}\int_{\tau_0}^{\tau}[b_1{}^0(\tau') - b_1{}^e(\tau')]\,d\tau' \quad \tau < \tau_0; \quad (32)$$

$$S_2{}^e(\tau) - S_1{}^0(\tau) = \frac{2}{u}\int_{\tau_{th}}^{\tau_0}[b_1{}^e(\tau') - b_2{}^e(\tau')]\,d\tau' + \frac{2}{u}\int_{\tau_0}^{\tau}[b_1{}^0(\tau') - b_2{}^e(\tau')]\,d\tau', \tau > \tau_{th}^e, \quad (33)$$

which follow from the relations $dS_\nu^e/d\tau = -2b_\nu^e(\tau)/u$ and the conditions:

$$S_1{}^0(\tau_0) = S_1{}^e(\tau_0), \quad S_2{}^e(\tau_{th}) = S_1{}^y(\tau_{th}).$$

It is obvious that the conditions for the applicability of the s.p. method are violated in the neighborhoods of the points τ_{th}^e and τ_0, at which the different branches of the scattering function merge and the quasi-classical formulas (30) and (31) give expressions which diverge (like $(\tau - \tau_0)^{-1/2}$ as $\tau \to \tau_0$ and like $(\tau - \tau_{th}^e)^{-1/4}$ as $\tau \to \tau_{th}^e$). Therefore, in each of these regions (regions I and II in Fig. 1b), it is necessary to obtain quantum expressions.

First we shall consider the vicinity of the point τ_{th}^e (region I), in which the derivation of $\Delta\rho(\tau)$ is completely analogous to that of formula (20) for the inelastic cross section. When $\tau \to \tau_{th}^e$, the quadratic expansion in (25) of the action $S^e(b, z, \tilde{z}, \tau)$ about the s.p. points, performed in calculating $\Delta\rho$ by the s.p. method, is no longer sufficient, since for $\tau = \tau_{th}^e$ the determinant of this quadratic form, equal to

$$\text{Det}\,\hat{D}^{(\nu)}_{b,z,\tilde{z}} = \frac{2}{u}\frac{d^2\tau_\nu{}^e}{db^2}\left(\frac{(z_\nu - \tilde{z}_\nu)\Delta F}{uR_0}\right)^2$$

vanishes. Expanding the action $S^e(b, z, \tilde{z}, \tau)$ up to the necessary third-order terms and performing the calculation, analogous to that of $\rho_{12}(\tau)$, of the corresponding integrals gives in the quantum region of angles (region I) the following expression for the cross section $\Delta\rho(\tau)$ in terms of the Airy function:

$$\Delta\rho = -\sqrt{\rho_1{}^0(\tau)}\,p(b_{th}^e)\,4\sqrt{\frac{\tau b_{th}^e}{u}}\left(\frac{\varkappa^e}{u}\right)^{-1/3}\Phi\left(-\frac{2}{u}\Delta\tau\left(\frac{\varkappa^e}{u}\right)^{-1/3}\right) \times\cos\left[\frac{S_1{}^e(\tau)+S_2{}^e(\tau)}{2} - S_1{}^0(\tau) - \frac{\pi}{4}\right], \quad (34)$$

where $\Delta\tau = \tau - \tau_{th}^e$, $b_{th}^e = b_1^e(\tau_{th}^e) = b_2^e(\tau_{th}^e)$, κ^e is defined after (29) and the meaning of the actions is the same as in (30) and (31). Using the asymptotic behavior of the function $\Phi(x)$ when $|x| > 1$, it can be shown that on decrease of the angles from the threshold value τ_{th}^e the increment $\Delta\rho$ to the elastic cross section, while continuing to oscillate, is damped exponentially in amplitude. On increase of τ from τ_{th}^e, the asymptotic form of $\Phi(x)$ and the relation

$$S_1{}^e(\tau) - S_2{}^e(\tau) \approx \frac{4}{3}\sqrt{2/\varkappa^e}\,(\tau - \tau_{th}^e)^{3/2}, \quad \tau \to \tau_{th}^e$$

bring (34) to the form

$$\Delta\rho = -\sqrt{\rho_1{}^0(\tau)\,b_{th}^e\tau}\,(2\varkappa^e\Delta\tau)^{-1/4}\,2p(b_{th})\sin\left[\frac{S_1{}^e - S_2{}^e}{2} - \frac{\pi}{4}\right] \times\cos\left[\frac{S_1{}^e + S_2{}^e}{2} - S_1{}^0 - \frac{\pi}{4}\right],$$

which coincides with (31) as $\tau \to \tau_{th}^e$, when

$$\rho_1(\tau) = \rho_2(\tau) = b_{th}^e\tau_{th}^e\frac{d}{d\tau}\left(\sqrt{\frac{2(\tau-\tau_{th}^e)}{\varkappa^e}}\right).$$

Thus, the quantum expression (34) correctly matches with the quasi-classical expression (31).

We shall now examine the quantum region II, the vicinity of the point τ_0. Adding the third-order terms, necessary in this region, to the quadratic expansion of the action in $\Delta b = b - R_0$, z, $\tilde{z}$ and $\Delta\tau = \tau - \tau_0$, we obtain for the action the expression

$$S^e = S_1^0(\tau_0) - \frac{2R_0}{u}\Delta\tau - \frac{2}{u}\Delta b\Delta\tau + \frac{\Delta F}{u}y\Delta b + \frac{1}{\beta u}(\Delta b)^2 + \frac{\Delta F}{4R_0}x^2 y;$$
$$x = (z+\tilde{z})/2;\quad y = z - \tilde{z};\quad \beta = db_1^0/d\tau|_{\tau_0}.$$

Calculation of the integral in (25) with the action indicated above in the region $b \sim R_0$, $\tau \sim \tau_0$ leads to an expression for the cross section in terms of the parabolic cylinder function $D_{-1/2}(x)$ (cf. the integral representation of this function in [14]):

$$\begin{aligned}\Delta\rho(\tau) &= 2\sqrt{\rho_1^0(\tau)\rho_2^y(\tau)}\\ &\times p(b_2^y(\tau))\cos[S_2^y - S_1^0\\ &+ \pi/2] - 2\rho_1^0(\tau)p(b=0)\\ &\times\sqrt{R_0}\,|2\beta u|^{-1/4}F\left(\Delta\tau\sqrt{\frac{2|\beta|}{u}}\right),\\ \Delta\tau &= \tau - \tau_0.\end{aligned} \tag{35}$$

Here $\beta = db_1^0/d\tau\,|_{\tau = \tau_0}$ and the function F(A) is equal to

$$F(A) = \mathrm{Re}\left\{\exp\left[-\frac{i\pi}{8} - \frac{iA^2}{4}\right]D_{-1/2}(e^{-i\pi/4}A)\right\}, \tag{36}$$

and is depicted in Fig. 4. The function F(A) oscillates for $A < 0$ and falls away monotonically for $A > 0$, with, for $|A| > 1.5$, the corresponding asymptotic forms:

$$F(A) = \begin{cases} A^{-1/2}, & A > 1.5,\\ (2/A)^{1/2}\cos\dfrac{A^2}{2}, & |A| > 1.5,\quad A < 0.\end{cases} \tag{37}$$

Using (37), one can show that the quantum expression (35) goes over to the quasi-classical expressions (30) or (31) as τ deviates from τ_0 in the direction of larger or smaller angles. In fact, the quantity $A^2/2$, which determines the phase of the slow oscillations in (35) upon which the rapid oscillations from the branch $b_2^e(\tau)$ are imposed, can be represented in the form

$$\left.\frac{A^2(\tau)}{2}\right|_{\tau\sim\tau_0} = \frac{2}{u}\int_{\tau_0}^{\tau}[b_1^0(\tau) - b_1^y(\tau)]\,d\tau \quad \text{for } \tau < \tau_0.$$

In a similar way, using (37) and the explicit form of $b_1^e(\tau)$ as $\tau \to \tau_0$, it is easy to verify the correct matching of the expressions (35) and (31) in the amplitude of the slow oscillations for $\tau < \tau_0$, and that of the expressions (35) and (30) in the magnitude of the non-oscillating term for $\tau > \tau_0$.

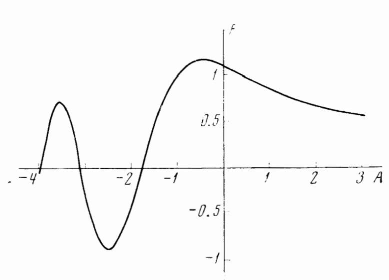

FIG. 4. The function F(A) (formula (40)) describing the elastic scattering in the quantum region II (cf. Fig. 1).

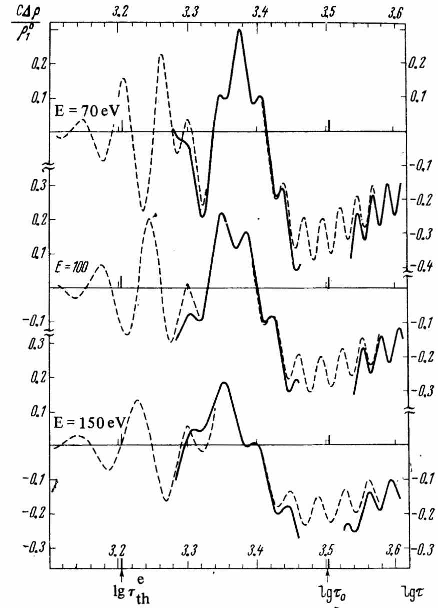

FIG. 5. The relative change $C\Delta\rho/\rho_1^0$ in the elastic cross-section $\rho_{11}(\tau)$ under the influence of transitions to an excited term. $C = 2R_0p_0/a$, $p_0 = p(b = 0)$.

Figure 5 shows the relative change $\Delta\rho/\rho_1^0(\tau)$, calculated from the formulas (30), (31), (34), and (35), ($\Delta\rho/\rho_1^0 \simeq \ln\rho_{11}(\tau) - \ln\rho_1^0$ for $\Delta\rho/\rho_1^0 \ll 1$), in the elastic cross section under the influence of an inelastic process, with the following parameters, which are close to the real situation in the He^+–Ne system:

$$\tau_{th}^e = 1600\ \text{eV-deg},\ \tau_0 = 3200\ \text{eV-deg},\ R_0 = b_1^0(\tau_0) = 1.61\ \text{at. un.} \tag{38}$$

For the function $b_1^0(\tau)$ we have used the theoretical dependence (from amongst those obtained in [1] by treatment of the elastic scattering data) that takes account of the polarization attraction. For the functions $b_1^e(\tau)$ and $b_2^e(\tau)$ we have used the approximation

$$\begin{aligned} b_1^e(\tau) &= R_0 - d + \frac{d}{2}\sqrt{t}(3-t);\\ b_2^e(\tau) &= R_0 - d + \frac{3d}{2}\sqrt{t};\quad t = \frac{\tau - \tau_{th}^e}{\tau_0 - \tau_{th}^e};\quad d = 0.3\ \text{at. un.}\end{aligned} \tag{39}$$

The formula (39) ensures the correct behavior of (29) at the threshold ($\tau = \tau_{th}^e$, $t = 0$) with the parameter $\kappa^e = {}^8/_9(\tau_0 - \tau_{th}^e)/d^2$, and the contact with the vertical at the point $\tau = \tau_0$ ($t = 1$) with curvature

$$\left.\frac{d^2b_1^e}{d\tau^2}\right|_{\tau_0} = -\frac{3}{4}\frac{d}{(\tau_0 - \tau_{th}^e)^2}. \tag{40}$$

From a comparison of (40) with (28), we find the value $\Delta F = 44$ eV/a.u. corresponding to the parameters chosen in (38) and (39). The dashed curve in Fig. 5 corresponds to a calculation from the quantum formulas (34) and (35) in the respective regions I and II; the solid curve is calculated from the quasi-classical formulas (30) and (31). Allowing for the approximate character of the formulas, the matching of these curves must be regarded as good.[3)] Moreover, the picture presented in the figure agrees qualitatively with the elastic scattering curves observed in [2] in the systems He^+–Ne and He^+–Ar.

From the above analysis and numerical calculations, we can draw the following conclusions, which are important for the interpretation of experimental anomalies in elastic scattering:

1) The oscillations in the elastic cross-section are already beginning at angles less than the threshold value τ_{th}^{e}; on the unperturbed elastic scattering curve $b_1^0(\tau)$, this value corresponds to the impact parameter value $b_c = b_1^0(\tau_{th}^{e})$, which does not coincide with the radius of intersection of the terms: $b_c > R_0$ (cf. Fig. 1b).

2) The angle τ_0, which corresponds to the intersection radius $R_0 = b_1^0(\tau_0)$, can be determined approximately from the dip in the curve for the elastic cross section.

3) The oscillations in the intermediate region of angles cannot be described by only one harmonic; for elastic scattering, this does not permit us to use a derivation of the same experimental function $N(\tau E)$ as in the inelastic scattering.

As we have since found out, results [16, 17] concerning differential cross-section features have been obtained which are analogous to ours in many respects and more general in the sense that they are not confined to high energies and small transition probabilities; the important point is that the non-monotonic character, described above, of the scattering functions determining the elastic and inelastic processes is conserved.

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[3)]The matching of the quantum and quasi-classical calculations at $\tau = \tau_{th}^{e}$ can be improved by using, in place of the approximation (34), the improved Airy approximation proposed in [15] for the description of rainbow scattering.

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220