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Time delay in atomic collisions

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The time delay, as defined via phase shifts, does not apply to atom-atom collisions because of the semiclassical nature of the system. In this limit the contribution of one partial wave to the cross section is negligible. Therefore, we analyze time delay for the scattering amplitude and show that some new phenomena may occur, which cannot be explained by the time delay for a single phase shift. The time delay, which is averaged over all scattering angles, shows structure corresponding to several delay mechanisms. We also show that the lifetime of a resonance state, formed in a collision, may be considerably shorter than expected from the theory of resonance scattering.

I. INTRODUCTION

The concept of time delay in collisions has been known for some time.[1,2] It was first defined in terms of phase shifts, primarily because in many applications of nuclear physics only a few partial waves are required to obtain the scattering amplitude. If the phase shift for the lth partial wave is known, it was shown that the time delay is

$$\tau_l = \hbar \frac{d\delta_l}{dE} . \tag{1.1}$$

Such a concept is also very convenient for defining the lifetime of a resonance, since it can be shown that one is just half of the other,[3] i.e., the lifetime is half of the time delay, for a resonance in a given partial wave.

Although time delay is a well-defined quantity, it has never actually been measured in a real experiment since such measurements are very difficult to perform. An exception occurs in high-energy physics where the delay time can be associated with the length of the trace that elementary particles (resonances) leave before disintegrating. However, for a very short-lived resonance such a trace is not visible and the lifetime is estimated from the half-width of the cross section.[4] This is again based on the assumption that scattering is dominated by only a few partial waves.

Rigorously speaking, the time delay (1.1) does not reflect reality. It would be more appropriate to ask what is the time delay for real experimental conditions? Under such circumstances, the resonance contributes only partially to the cross section, hence the real time delay measured at a certain angle θ will be different than that given by (1.1). In atomic collisions this is just the case: Many partial waves are required for an accurate description of the differential cross section and if there is a resonance, its contribution is mixed with other effects which are more dominant.[5,6] Therefore, a more accurate definition of time delay would be obtained via the scattering amplitude. It can be shown that in such a case,[7]

$$\tau_\theta = \hbar \frac{d}{dE} \arg[f(\theta)] = \frac{\hbar}{|f|^2} \operatorname{Im}\left(f^* \frac{df}{dE}\right), \tag{1.2}$$

where $f(\theta)$ is the scattering amplitude. Such a delay is angle dependent, and describes the real situation. Again, if only a few partial waves are enough to determine $f(\theta)$ it can easily be shown that (1.2) reduces to (1.1). For such a definition of time delay the results obtained from (1.1) no longer apply. For example, in atom-atom collisions we find that the solutions of (1.1) and (1.2) are identical only for extremely narrow resonance and large-angle scattering. However, as soon as the resonance becomes wider or if we calculate τ_θ in the forward direction, where diffraction is dominant, we would find deviations from the results obtained by using (1.1). In Sec. II we discuss the time delay τ_θ for $\theta = 180°$. This is an example where, at low energy, the resonance cross section is dominant (backward glory) while at high energy it disappears and only the direct reflection cross section is present. At low energy and exactly at the resonance energy we find the time delay is similar to that obtained from (1.1), however, with some additional terms which can be neglected to a certain extent. As the energy is increased the resonances contribute less to the cross section and so the deviation from (1.1) becomes more apparent. However, as will be shown, entirely new phenomen may occur. The time delay may become so negative, as in our example, that the low bound for (1.1), as discussed by Wigner,[1] cannot hold any longer. Such a phenomenon is accompanied by a small cross section, which is due to interference between the resonance amplitude and the direct reflection amplitude. Even allowing for some averaging of the time delay over energy spread, we still obtain a large negative delay.

The description of (1.2) is given in the Regge representation of the scattering amplitude, appropriately modified to take into account the hard core in the atom-atom potentials. Such a representation allows a simple yet accurate separation of resonance contributions and that of direct reflection. The difficulty with the definition (1.2) of the time delay is twofold: (a) It is angle dependent, hence it is not a quantity characteristic of collisions, and (b) it is very difficult to measure. Therefore, it is more natural to define an averaged time delay which can be more easily related to the measurements. We define $\bar{\tau}$ by

$$\bar{\tau}=\frac{1}{\sigma}\int_{4\pi}\sigma(\theta)\tau_\theta d\Omega\ , \tag{1.3}$$

where σ is the total cross section. In fact, it is this quantity which is measured in high-energy physics in the case of short-lived resonances. In atomic collisions $\bar{\tau}$ is important for studies of the recombination process, observation of resonances in plasma and in general for cases when a knowledge of the duration of collision is necessary for understanding or predicting collision-induced events.

As the first result of salving (1.3) we notice that, at least for atomic collisions, the relationship between the width of a resonance and its lifetime is no longer valid. The time delay is much shorter than that given by (1.1). Since the diffraction mode of scattering is dominant we will also rarely observe a large negative delay, which was found in τ_θ. As we have said, such a delay is associated with the fact that $\sigma(\theta)$ can be very small and this seldom occurs for σ.

In Sec. III we discuss $\bar{\tau}$ for which a complex angular momentum analysis is developed, similar to that for the scattering amplitude.[8] The example of Sec. II is also discussed with respect to $\bar{\tau}$. We find a general agreement with the theory based on (1.1), but the delay times are much shorter. We also find a negative delay, but this is mainly due to interference effects between the phase of residues and the poles of the S matrix. In fact, this negative delay is relatively large if we consider that the positive delay of narrow resonances is small.

II. TIME DELAY IN DIFFERENTIAL CROSS SECTIONS

As we have discussed in the Introduction, an experimental study of time delay in differential cross sections is difficult, but can reveal some interesting features about the mechanism of scattering. To study these effects we will use the well-known formula for time delay in a specified direction θ:

$$\tau_\theta=\frac{\hbar}{|f|^2}\,\mathrm{Im}\left(f^*\frac{df}{dE}\right), \tag{2.1}$$

or if one uses the usual units whereby E is replaced by $k^2=(2\mu/\hbar^2)E$, and k is in the units of $\mathrm{\AA}^{-1}$, we have for τ_θ:

$$\tau_\theta=\frac{\mu}{|f|^2}\,\mathrm{Im}\left(f^*\frac{df}{dk^2}\right)3.149\times10^{-13}\ (\mathrm{sec})\ , \tag{2.2}$$

where μ is the reduced mass in atomic mass units. The number that we obtain for τ_θ does not give a lot of information if it is not compared with another quantity, such as the distance that a particle travels during the time delay τ_θ before it escapes the interaction region. Therefore, we define a dimensionless quantity d defined by

$$d=\frac{\tau_\theta v}{r_0}=\frac{1}{r_0}\frac{1}{\sigma(\theta)}\,\mathrm{Im}\left(f^*\frac{df}{dk}\right), \tag{2.3}$$

where r_0 is the equilibrium position of the potential and v is the velocity of free particle.

The relationship (2.3) tells us how many times, during the time τ_θ, a free particle can travel the distance r_0. Although such a quantity is arbitrary, it will give us some information about the time delay (2.1). To study the time delay in atomic collisions we use a suitable representation of the scattering amplitude[8] which enables us to observe the effects of resonances, direct reflection, etc. In such a representation, the scattering amplitude $f(\theta)$ is

$$f(\theta)=\frac{1}{k}\int_0^\infty d\lambda\,\lambda S(\lambda)e^{-i\pi\lambda}P_{\lambda-1/2}(-\cos\theta) -\frac{\pi i}{k}\sum_n\lambda_n\beta_n\frac{P_{\lambda_n-1/2}(-\cos\theta)}{\cos(\pi\lambda_n)}\ , \tag{2.4}$$

where λ_n and β_n are the Regge poles and appropriate residues of the S matrix $S(\lambda)$, respectively. The most pronounced effect of resonances on the differential cross section is backward glory,[9] therefore we will study the time delay for $\theta=\pi$. We could have taken any other angle but that would not contribute more to our understanding of $\tau(d)$. For simplicity we will restrict our discussion only to the contribution of one pole to the scattering amplitude. We justify such an approximation by noting that the contribution of each pole to the scattering amplitude is proportional to[9] $\exp[-\pi\,\mathrm{Im}(\lambda_n)]$ for $\theta=\pi$. Therefore, at high energy, when all the poles have large imaginary parts, we obtain an accurate description of the scattering amplitude by only retaining the pole with the smallest imaginary part. At low energy several poles may equally contribute to $f(\theta=\pi)$, hence, we expect deviation from one pole approximation.

The integral in (2.4) can be evaluated analytically,[8] hence $f(\pi)$ is

$$f(\pi)=f_B+f_R=\frac{i}{k}\left(\frac{e^{2i\eta_0}}{2\eta_0''}-\pi\frac{\lambda_1\beta_1}{\cos(\pi\lambda_1)}\right), \qquad (2.5)$$

where η_0 is the phase shift and $\eta_0''=d^2\eta_0/d\lambda^2$, both evaluated for $\lambda=0$. For high energy, the imaginary part of λ_1 is large, in which case the direct reflection term is dominant

$$f_B(\pi)=\frac{i}{k}\frac{e^{2i\eta_0}}{2\eta_0''}, \qquad (2.6)$$

while for low energy, when $\text{Im}(\lambda_1)\sim 0$, the dominant term in (2.5) is

$$f_R=-\frac{i\pi}{k}\frac{\lambda_1\beta_1}{\cos(\pi\lambda_1)}. \qquad (2.7)$$

Thus the time delay will behave differently in these two limiting cases. Let us first see what will be the time delay with only direct reflection waves. By taking a derivative of (2.6) with respect to energy and then calculating (2.1) we find

$$\tau\equiv\tau_\pi=\frac{4\mu}{\hbar}\frac{d\eta_0}{dk^2}. \qquad (2.8)$$

The phase shift η_0 can be calculated from the WKB approximation, in which case we obtain from (2.8) the classical time delay for a particle colliding "head on" with the target. We would obtain a negative delay since the particle "saves" twice the distance between the hard core and the center of the target. In addition the particle travels faster than the free particle due to the attractive action of the potential. Therefore, d is negative and of the order of $d\sim-2$.

At low energy the Regge term is dominant. We find

$$\tau=\frac{2\mu}{\hbar}\left[\text{Im}\left(\frac{\lambda_1^0}{\lambda_1}\right)+\text{Im}\left(\frac{\beta_1^0}{\beta_1}\right)+\pi\,\text{Im}[\lambda_1^0\,tg(\pi\lambda_1)]\right], \qquad (2.9)$$

where the circle indicates a derivative with respect to k^2.

When $\text{Im}(\lambda_1)$ is small and $\text{Re}(\lambda_1)$ an integer, we have an estimate,

$$\lambda_1^0\sim\text{Re}(\lambda_1^0),\quad \tan(\pi\lambda_1)\sim 0, \qquad (2.10)$$

therefore

$$\tau\sim\frac{2\mu}{\hbar}\text{Im}\left(\frac{\beta_1^0}{\beta_1}\right). \qquad (2.11)$$

From the unitarity of the S matrix

$$S=\frac{\lambda-\lambda_1^*}{\lambda-\lambda_1}e^{2i\alpha}, \qquad (2.12)$$

where α is the background phase, we find approximate β_1:

$$\beta_1\sim 2ie^{2i\alpha}\,\text{Im}(\lambda_1) \qquad (2.13)$$

which gives for τ

$$\tau\sim\frac{4\mu}{\hbar}\alpha^0. \qquad (2.14)$$

From the WKB approximation for $\text{Im}(\lambda_1)$ (Ref. 8) we can calculate α and obtain the zero delay for τ. This corresponds to the fact that the particle does not penetrate the centrifugal barrier formed by $V+\lambda_0^2/R^2$, but is flying without being deflected (in this derivation we have assumed that V can be neglected at the outermost turning point). On the other hand, when $\text{Re}(\lambda_1)$ is a half-integer, we have

$$\tan(\pi\lambda_1)\sim\frac{i}{2\pi\,\text{Im}(\lambda_1)}, \qquad (2.15)$$

in which case

$$\tau\sim\frac{2\mu}{\hbar}\left(2\alpha^0+\frac{1}{2}\frac{\text{Re}(\lambda_1^0)}{\text{Im}(\lambda_1)}\right)\sim\frac{\mu}{\hbar}\frac{\text{Re}(\lambda_1^0)}{\text{Im}(\lambda_1)}, \qquad (2.16)$$

which is large and positive since $\text{Im}(\lambda_1)$ is small. This is the well-known result if α^0 can be neglected.[10] Incidentally, this large value for time delay corresponds to a large total cross section.

For high energy, when $\text{Im}(\lambda_1)$ is large, we can replace $\tan(\pi\lambda_1)$ by i and find for (2.9):

$$\tau\sim\frac{2\mu}{\hbar}\left[\text{Im}\left(\frac{\lambda_1^0}{\lambda_1}+\frac{\beta_1^0}{\beta_1}\right)+\pi\,\text{Re}(\lambda_1^0)\right]\sim\frac{2\mu}{\hbar}\pi\,\text{Re}(\lambda_1^0). \qquad (2.17)$$

Hence, the time delay is positive since the poles move towards larger values of $\text{Re}(\lambda_1)$ for increasing energy. However, in contrast to the low-energy case, the time delay is now smooth. This can be understood in terms of clockwise and anticlockwise waves which were discussed in the context of the differential cross section.[9] If both waves live long enough to travel around the target several times, as is the case at low energy, their superposition can form a standing wave, thus enhancing their lifetime. Otherwise they are just traveling decaying waves with a positive lifetime given by (2.17).

It is interesting to calculate the lifetime of the resonance waves at high energy and at an arbitrary angle θ. By using the approximation of f_R for large $\text{Im}(\lambda_1)$, we find

$$\tau_\theta\sim\frac{2\mu}{\hbar}\theta\,\text{Re}(\lambda_1^0), \qquad (2.18)$$

then (2.17) is a special case of (2.18) for $\theta=\pi$. Therefore we can define the angular velocity of the traveling waves by

$$\omega_R=\frac{\hbar}{2\mu}\frac{1}{\text{Re}(\lambda_1^0)} \qquad (2.19)$$

from which we get the corresponding angular momentum

$$\hbar\,\mathrm{Re}(\lambda_1) = I\,\omega_R = \frac{\hbar r^2}{2\,\mathrm{Re}(\lambda_1^0)} \qquad (2.20)$$

where I is the momentum of inertia of the particle and r is some mean radius. r is almost constant over a large variation in energy, hence

$$\mathrm{Re}(\lambda_1) \sim kr\,, \qquad (2.21)$$

which indicates that $\mathrm{Re}(\lambda_1)$ is a linear trajectory, a fact confirmed in many calculations. The results of (2.19)–(2.21) are outside our main interest, but are given to illustrate the physical meaning of the Regge poles.

The relationship (2.17) gives the time when we observe the f_R waves if it is not decaying. However, the f_R wave decays and the rate of its decay is determined by the value of $\mathrm{Im}(\lambda_1)$. For large $\mathrm{Im}(\lambda_1)$ the amplitude of f_R is small. Since for $\theta=\pi$ the scattering amplitude is given as the sum (2.5) for large $\mathrm{Im}(\lambda_1)$ the f_B amplitude is dominant. Therefore, the real time delay is no longer given by (2.17) but by (2.8), i.e., it is negative. For low energy, when f_R is dominant, the time delay is given by (2.16). Owing to interference between f_B and f_R at low energy, the time delay is not zero for $\mathrm{Re}(\lambda_1)$ = integer, but negative and approximately as given by (2.8).

The time delay at $\theta=\pi$ was calculated, in one pole approximation for a model system with the potential

$$V = V_0\left(\frac{r_0}{r}\right)^6\left[\left(\frac{r_0}{r}\right)^6 - 2\right], \qquad (2.22)$$

where the parameters are $V_0 = 0.458$ eV and $r_0 = 1.74$ Å (the parameters for the H–Hg system). The range of energy is $E = 0.17 - 0.87$ eV, which bridges two extreme cases; when backward glory is dominant and when f_B is dominant. The Regge poles were calculated numerically.[11] The imaginary part of λ_1 varies from $\mathrm{Im}(\lambda_1) = 0.005$ at low energy to $\mathrm{Im}(\lambda_1) = 3.25$ at high energy. Table I is of the Regge poles and corresponding residues and shows some of their calculated values. The

TABLE I. The values of the Regge pole λ_1 and the corresponding residue for different energies which were used in the calculation of time delay.

E (eV)	λ_1	β_1
0.18	$29.720 + i\,0.005$	$0.002 + i\,0.017$
0.19	$30.051 + i\,0.01$	$-0.003 + i\,0.022$
0.20	$30.383 + i\,0.017$	$-0.013 + i\,0.033$
0.25	$32.026 + i\,0.112$	$-0.251 + i\,0.064$
0.33	$34.495 + i\,0.436$	$-1.338 - i\,0.629$
0.41	$36.73 + i\,0.856$	$-3.299 - i\,2.661$
0.62	$41.542 + i\,1.977$	$-13.793 - i\,12.539$
0.87	$46.358 + i\,3.247$	$-37.476 - i\,25.841$

effective radius r in (2.21) was also calculated and it varies from $r = 1.98 - 1.86$ Å, i.e., it is almost constant.

In Fig. 1 we show the results of calculation for d (solid line). In addition we show d_R and d_B. As expected d_B is almost constant and if divided by 2, we find the approximate point of the closest approach of two atoms (this point is in fact larger than the real one because the atoms travel faster in the attractive part of the potential). The line for d_R is also constant for high energy but almost coincides with the real d for low energy. However, the real d shows interesting behavior. For low energy it follows a line which is expected from the theory of resonances. The peaks in d coincide with the rise of the cross section. However, in the case of intermediate energy it does not follow either the line d_R or d_B. This oscilla-

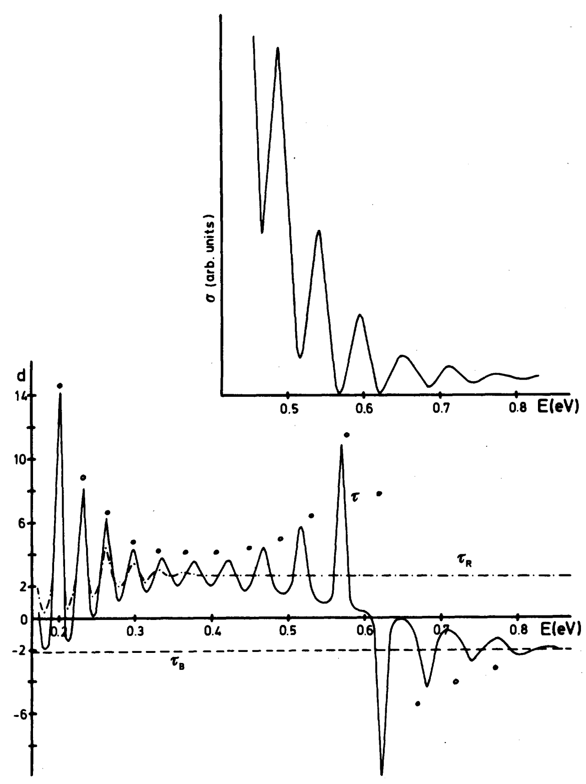

FIG. 1. Time delay $\tau_{\theta=\pi}$ (solid line) calculated in the energy range from the dominant resonance to the dominant direct reflection scattering in the differential cross section. The resonance structure is described by a single Regge pole from Table I. Differential cross section for $\theta=\pi$ is also inserted for correlation with peaks in time delay. At lower energy the peaks in time delay correspond to the peaks in differential cross section. The time delay for the direct reflection (------) and resonance (-·-·-·-) waves is also given. The unit d on the abcissa is explained in the text. The circles indicate positions of $\mathrm{Re}(\lambda)$ = half-integer.

tory behavior is entirely due to the interference between f_R and f_B. There is also a dramatic reversal of behavior of peaks. The large values of d correspond to the minima of the total cross section, as shown in Fig. 1.

There is an unusual phenomena in d. For a certain energy, the time delay is considerably negative, as the atoms are reflected from each other before they even make contact. In Fig. 1 this happens at $E \sim 0.62$ eV. However, the large negative delay is accompanied by a small, almost zero, cross section. Hence, the "nonphysical" behavior is balanced out by the fact that there are no observable particles with such behavior. However, when the cross section is averaged over a small interval of energy, in the neighborhood of the one for which $\sigma \sim 0$ we get a small flux of particles with a large negative delay, larger than the mean radius of the potential. The behavior of d for high energy is as predicted; it goes over to d_B.

III. AVERAGE TIME DELAY

The quantity which is treated here is the average time delay. The question arises: If two particles collide, what would be the most probable time delay for scattering? As we saw in the previous section, sometimes a large time delay may correspond to a small cross section, therefore some averaging is necessary since it is obvious that such a state is not very probable.

We define the average time delay by

$$\bar{\tau} = \frac{1}{\sigma}\int \sigma(\theta)\tau_\theta d\Omega \,, \tag{3.1}$$

where σ is the total cross section. By replacing τ_θ with (2.1) and using a partial-wave expansion of the scattering amplitude, we obtain

$$\bar{\tau} = \frac{\pi\hbar}{\sigma k^2}\,\mathrm{Im}\left(\sum_l (2l+1)\mathring{S}_l(S_l^* - 1)\right), \tag{3.2}$$

where the circle designates a derivative with respect to E. It can be easily shown that

$$\bar{\tau} = \frac{4\pi\hbar}{\sigma k^2}\sum_l (2l+1)\mathring{\delta}_l \sin^2\delta_l \,, \tag{3.3}$$

which can be identified as

$$\bar{\tau} = \frac{4\pi\hbar}{\sigma k^2}\,\mathrm{Im}\left(\frac{1}{i}\sum_l (2l+1)\mathring{\delta}_l(S_l - 1)\right). \tag{3.4}$$

Therefore, we can define an amplitude F by

$$F = \sum_l (2l+1)\mathring{\delta}_l(S_l - 1)\,, \tag{3.5}$$

whence the average time delay is

$$\bar{\tau} = \frac{4\pi\hbar}{\sigma k^2}\,\mathrm{Im}\left(\frac{1}{i}F\right). \tag{3.6}$$

Formally, (3.5) is similar to the scattering amplitude in the forward direction except for $\mathring{\delta}_l$, which is given by

$$\mathring{\delta}_l = \frac{1}{2i} S_l^{-1}\mathring{S}_l \,. \tag{3.7}$$

The derivative of the phase shift has some useful properties. It is a symmetrical function with respect to $l \to -l$. Furthermore, it has first-order poles in the first quadrant and it also has poles in the fourth quadrant of the complex l plane. This can be easily shown from the unitarity property of the S matrix

$$S_\lambda^{-1} = S_{\lambda^*}^* \tag{3.8}$$

and if S_λ has a pole λ_n in the first quadrant, then S_λ has a zero in the fourth, given by λ_n^*. Hence S_λ^{-1} has poles at λ_n^*. If we parametrize S_λ near the pole by

$$S_\lambda \sim \frac{\beta_n}{\lambda - \lambda_n} \tag{3.9}$$

then we easily find that

$$S_\lambda^{-1}\mathring{S}_\lambda \sim \frac{\mathring{\lambda}_n}{\lambda - \lambda_n} \tag{3.10}$$

and

$$S_{\lambda^*}^{-1}\mathring{S}_{\lambda^*} \sim -\frac{\mathring{\lambda}_n^{*}}{\lambda^* - \lambda_n^*}\,. \tag{3.11}$$

By reviewing these properties of $\mathring{\delta}_l$, we can proceed to evaluate F. We can use the Poisson summation formula[12] to transform F into

$$F = 2\sum_{m=-\infty}^{\infty} (-)^m \int_0^\infty d\lambda\, \lambda \mathring{\delta}_\lambda (S_\lambda - 1) e^{2im\pi\lambda}. \tag{3.12}$$

The sum can be split into three parts: One for negative, one for positive, and one with $m = 0$. We can also sum over all the indices in the first two parts and obtain

$$F = 2\int_0^\infty d\lambda\,\lambda\mathring{\delta}_\lambda(S_\lambda - 1) - 2\int_0^\infty d\lambda\,\lambda\mathring{\delta}_\lambda(S_\lambda - 1)\frac{e^{2i\pi\lambda}}{1+e^{2i\pi\lambda}}$$

$$-2\int_0^\infty d\lambda\,\lambda\mathring{\delta}_\lambda(S_\lambda - 1)\frac{e^{-2i\pi\lambda}}{1+e^{-2i\pi\lambda}}\,. \tag{3.13}$$

The first integral will be evaluated later, but now we turn our attention to the last two. In the second integral we can distort the integration path, which is slightly above the positive real axis, to the imaginary axis. In that case, we get a contribution from the poles of $\mathring{\delta}_\lambda$ and S_λ. We find for this integral

$$\int_0^\infty = -\int_0^\infty d\lambda\,\lambda\delta^0_{i\lambda}(S_{i\lambda}-1)\frac{e^{-2\pi\lambda}}{1+e^{-2\pi\lambda}}$$
$$+\pi\sum_n \frac{\beta_n\lambda_n^0}{1+e^{-2i\pi\lambda_n}}\left(1+2i\pi\lambda_n\frac{e^{-2i\pi\lambda_n}}{1+e^{-2i\pi\lambda_n}}\right)$$
$$-\pi\sum_n\frac{\lambda_n\lambda_n^0}{1+e^{-2i\pi\lambda_n}}\,, \qquad (3.14)$$

where we have used (3.10) and

$$S^0_\lambda \sim -\frac{\lambda_n^0\beta_n}{(\lambda-\lambda_n)^2}\,. \qquad (3.15)$$

In the third integral of (3.13) the line of integration can be shifted to the negative imaginary axis, in which case we must use (3.11). We find

$$\int_0^\infty = -\int_0^\infty d\lambda\,\lambda\delta^0_{i\lambda}(S_{i\lambda}e^{2\pi\lambda}-1)\frac{1}{1+e^{2\pi\lambda}}$$
$$-\pi\sum_n\frac{\lambda_n^*\lambda_n^{0*}}{1+e^{2i\pi\lambda_n^*}}\,, \qquad (3.16)$$

where we have used the symmetry property for S_λ:

$$S_{-\lambda}=e^{-2i\pi\lambda}S_\lambda\,. \qquad (3.17)$$

Finally, we have for F

$$F=2\int_0^\infty d\lambda\,\lambda\delta^0_\lambda(S_\lambda-1)+2\int_0^\infty d\lambda\,\lambda\delta^0_{i\lambda}\left(S_{i\lambda}-\frac{2}{1+e^{2\pi\lambda}}\right)$$
$$+4\pi\,\mathrm{Re}\left(\sum_n\frac{\lambda_n\lambda_n^0}{1+e^{-2i\pi\lambda_n}}\right)$$
$$-2\pi\sum_n\frac{\beta_n\lambda_n^0}{1+e^{-2i\pi\lambda_n}}\left(1+\frac{2i\pi\lambda_n}{1+e^{2i\pi\lambda_n}}\right)\,. \qquad (3.18)$$

The first integral in (3.18) is similar to the one obtained in the evaluation of the total cross section, except for δ^0_λ. However, it can be evaluated under the same assumptions, i.e., the integral gets most contributions from $\lambda\gg1$ and from the stationary point of $\arg(S_\lambda)$. In the first case, if we assume a potential with the tail $V\sim ar^{-S}$, then $\delta_\lambda\sim\alpha\lambda^{1-S}$, hence

$$\int_0^\infty d\lambda\,\lambda\delta^0_\lambda(S_\lambda-1)=\frac{2i}{S-1}\,\alpha^0\Gamma\left(\frac{4-2S}{1-S}\right)\times\alpha^{-(3-S)/(1-S)}\,e^{i\pi(2-S)/(1-S)}\,. \qquad (3.19)$$

Similarly we obtain for the stationary point of $\arg(S_\lambda)$

$$\int_0^\infty d\lambda\,\lambda\delta^0_\lambda(S_\lambda-1)=\delta^0_{\lambda_0}\lambda_0\left(\frac{\pi}{|\delta''_{\lambda_0}|}\right)^{1/2}e^{2i\delta_{\lambda_0}-i\pi/4}\,. \qquad (3.20)$$

The integral (3.19) can be associated with the time delay for diffraction waves while (3.20) can be associated with the delay for the forward glory waves. Before discussing them further, let us look at the second integral in (3.18). We find

$$\int_0^\infty\sim\eta_0^0\left(\frac{1}{\pi^2}e^{2i\eta_0}-\frac{1}{24}\right), \qquad (3.21)$$

where $\eta=\delta-\pi\lambda$. In the derivation of (3.21) we have used the approximation $\delta_{i\lambda}\sim i\pi\lambda+2\eta_0$, where $\eta_0=\eta\ (\lambda=0)$. This term, if it is compared with (2.8), can be associated with the averaged time delay arising from direct reflection. The remaining terms in (3.18) are due to resonances and will be discussed in the following section. Having F, we can now calculate $\bar\tau$. However, for this we need σ, which is given by[6]

$$\sigma=\frac{4\pi}{k^2}\left[\tfrac{1}{2}(2\alpha)^{2/S-1}\Gamma\left(\frac{3-S}{1-S}\right)\sin\left(\frac{\pi}{2}\,\frac{3-S}{1-S}\right)\right.$$
$$-\lambda_0\left(\frac{\pi}{|\delta''_{\lambda_0}|}\right)^{1/2}\sin(2\delta_{\lambda_0}+\tfrac{1}{4}\pi)$$
$$\left.-\pi\,\mathrm{Im}\left(\sum_n\lambda_n\beta_n\frac{e^{i\pi\lambda_n}}{\cos(\pi\lambda_n)}\right)\right], \qquad (3.22)$$

where

$$\alpha=\frac{\sqrt{\pi}}{4}\,\frac{\Gamma(S/2-1/2)}{\Gamma(S/2)}ak^{S-2}\,. \qquad (3.23)$$

IV. DISCUSSION

Let us now look at the properties of the averaged time delay. First, we will look at the contribution of separate (or partial) time delays, obtained in the previous section. As shown, F is given as a sum

$$F=F_{\rm diff}+F_{\rm fg}+F_{\rm dr}+F_r\,, \qquad (4.1)$$

where the indices stand for diffraction, forward glory, direct reflection, and resonances, respectively. Since the total cross section σ is also parametrized in such a way, it is reasonable to ask what is the property of the partial time delay, defined by

$$\bar\tau_p=\frac{4\pi\hbar}{\sigma_p k^2}\,\mathrm{Im}\left(\frac{1}{i}F_p\right), \qquad (4.2)$$

where the index p stands for either of the indices in (4.1). Let us first look at diffraction. We can easily find that

$$\bar\tau_{\rm diff}=\frac{2\mu}{\hbar}\,\frac{(S-2)(S-3)}{(S-1)^2}\,2^{2(S-2)/(S-1)}\cot\left(\frac{\pi}{2}\,\frac{3-S}{1-S}\right)\frac{1}{k^2}\,. \qquad (4.3)$$

The interesting feature of $\bar\tau_{\rm diff}$ is that it is independent of the detailed form of potential but only depends on the power with which the potential goes to zero for a large r. We also notice that $\bar\tau_{\rm diff}$ is positive. In the model case of Sec. II we find that

d, defined by (2.3), ranges from $d = 0.136$ to $d = 0.06$ in an energy interval $E = 0.17 - 0.87$ eV. Therefore the contribution of diffraction to the overall time delay is positive and smooth, but negligible.

The next contribution is τ_{fg}. We find

$$\bar{\tau}_{fg} = 2\hbar\delta^0_{\lambda_0} = \frac{2\mu}{\hbar}\frac{d(2\delta_{\lambda_0})}{dk^2}. \tag{4.4}$$

From the WKB approximation we can prove that $\bar{\tau}_{fg}$ is negative and of the order of the time delay for the direct reflection (2.8), and hence it is substantial. To illustrate this on the previous example, we find that d ranges from $d = -2.1$ to -1.32.

The averaged direct reflection time delay can also be calculated, however, in the definition of σ, given by (3.22), the appropriate term is not given. In the original derivation it was neglected.[8] If it is taken properly into account, we find

$$\bar{\tau}_{dr} = \frac{2\mu}{\hbar}\frac{d(2\eta_0)}{dk^2}, \tag{4.5}$$

which is exactly the delay for the backward scattering (2.8). The remaining term is the contribution of resonances. Here we develop an exercise to show the features of time delay produced by a single resonance; therefore we will restrict our discussion to one pole and look at two limiting cases: The low-energy [i.e., $\text{Im}(\lambda_1) \sim 0$] and the high-energy case [i.e., $\text{Im}(\lambda_1) \gg 1$]. As was already discussed, at the low energy such an approximation for the real time delay is poor, which is not the case at high energy. In the first case we can specify $\text{Re}(\lambda_1)$ to be either an integer or a half-integer. Therefore we have the following three cases.

i. $Im(\lambda_1) \sim 0$: $Re(\lambda_1)$ = integer.

$$F \sim 2\pi\,\text{Re}(\lambda_1)\,\text{Re}(\lambda_1^0) \tag{4.6}$$

from where we obtain

$$\bar{\tau}_r \sim 2\hbar\frac{\text{Re}(\lambda_1^0)}{\text{Im}(\beta_1)} \tag{4.7}$$

which is large since $\beta_1 \sim \text{Im}(\lambda_1)$.

ii. $Im(\lambda_1) \sim 0$: $Re(\lambda_1)$ = half-integer.

$$F \sim -\frac{2}{\text{Im}(\lambda_1)}\,\text{Re}(\lambda_1)\,\text{Re}(\lambda_1^0)(1 + e^{2i\alpha}), \tag{4.8}$$

hence $\bar{\tau}_r$ is

$$\bar{\tau}_r \sim \hbar\frac{\text{Re}(\lambda_1^0)}{\text{Im}(\lambda_1)}\,\frac{1 + \cos 2\alpha}{\cos 2\alpha}, \tag{4.9}$$

which is similar to the previous case.

iii. $Im(\lambda_1) \gg 1$. In such a case F is approximately zero, however, by dividing by σ_r we obtain a finite time delay.

In the discussion of these three cases, as well as discussing $\bar{\tau}_{fg}$ and $\bar{\tau}_{dr}$ we have assumed that these effects are the most dominant in σ. Since this is not the case, we get results which are not physical, such as the large time delay in *i* and a nonzero delay in *iii*. Purely from physical intuition we cannot expect this to happen. For example, in case *i* the cross section σ_r is negligible to other contributions in σ, hence we cannot divide F_r by σ_r. This is also the case with the other contributions to σ. It would be more appropriate to divide each F_p by σ_{diff} since this is dominant term in the total cross section. In order to see the value of such an approximation, we can compare σ_{diff} with the other contributions to the cross section. In particular we can compare σ_{diff} with the resonance cross section, since the resonance have a most interesting time delay behavior.

From (3.22) and assuming a very narrow resonance [i.e., $\text{Im}(\lambda_1) \sim 0$], the maximum of σ_r is given by

$$\sigma_r^{\max} \sim \frac{8\pi}{k^2}\,l, \tag{4.10}$$

where $l = \text{Re}(\lambda_1 - \frac{1}{2})$. If we now assume that the potential for a large r is of the form $V \sim -2V_0 r_0^6 r^{-6}$, we get for the ratio $\sigma_r/\sigma_{\text{diff}}$:

$$\sigma_r/\sigma_{\text{diff}} \sim \frac{l}{3(V_0 r_0^6 k^4)^{2/5}}, \tag{4.11}$$

which is always small. Similarly we obtain for the potentials $V \sim -2V_0 r_0^4 r^{-4}$

$$\sigma_r/\sigma_{\text{diff}} \sim \frac{l}{5(V_0 r_0^4 k^2)^{2/3}}. \tag{4.12}$$

From such estimates, we can now calculate $\bar{\tau}_r$, defined by

$$\bar{\tau}_r = \frac{4\pi\hbar}{k^2}\,\frac{\text{Im}(1/iF_r)}{\sigma_{\text{diff}}}. \tag{4.13}$$

In such a case the averaged resonance time delay is zero in cases *i* and *iii*. However, in case *ii* we obtain

$$\bar{\tau}_r \sim \frac{4\pi\hbar}{k^2}\,\frac{1}{\sigma_{\text{diff}}}\,\frac{2\,\text{Re}(\lambda_1)\,\text{Re}(\lambda_1^0)}{\text{Im}(\lambda_1)}\,[1 + \cos(2\alpha)], \tag{4.14}$$

where we have used the estimate (2.13). If we use (4.10) and (2.16), the time delay (4.14) simplifies further to

$$\bar{\tau}_r \sim 4\frac{\sigma_r^{\max}}{\sigma_{\text{diff}}}\,\tau\cos^2\alpha, \tag{4.15}$$

which shows that the averaged resonance delay is essentially determined by the ratio of the total

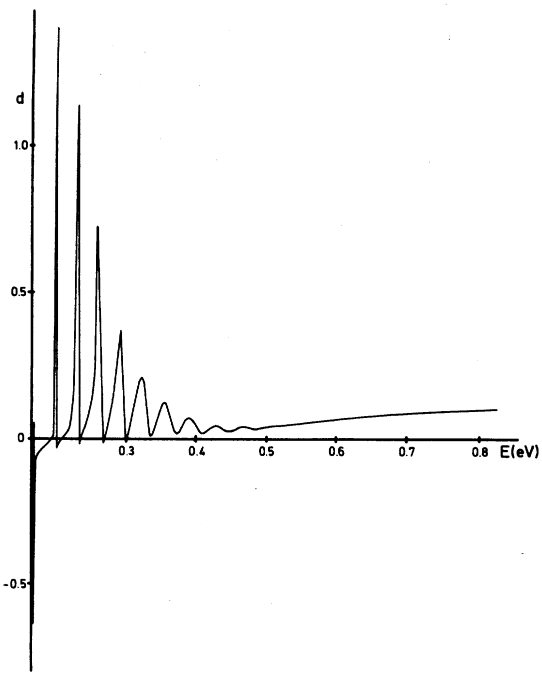

FIG. 2. The averaged time delay $\bar{\tau}$ is shown in the same energy range as in Fig. 1. The peaks correspond to the resonances, while the negative time delay at low energy is an interference effect and is positioned slightly above the positive resonance time delay. The unit d is explained in the text.

resonance and diffraction cross sections. From (4.11) and (4.12) we conclude that $\bar{\tau}_r$ is much smaller than the true resonance lifetime. The time delay can even be zero if the background phase α of the residue is $\pi/2$, which is an interesting phenomena not present if one only considers the time delay for one partial wave.

The true time delay τ is, as we have already mentioned, greatly reduced in a collision due to the fact that most of the scattering comes from the tail of the potential, i.e., diffraction scattering is most probable. Therefore, in a real collision such as an atom-atom collision, we cannot use the classical theory of the lifetime of resonances, especially for predicting the lifetime of states formed in such a collision. At best we can say that such long-lived states have lifetimes of the order of one-half of that given by (4.15).

In Fig. 2 we show results of calculations for $\bar{\tau}$ in the same system as discussed in Fig. 1. The energy range is also the same. We find a good correlation with the resonance cross section, i.e., a long delay corresponds to a large cross section. However, if we compare Fig. 2 with Fig. 1 we notice that d is much smaller in Fig. 2. It is almost one order of magnitude smaller. This is entirely due to the fact that σ_{diff} is in fact the most dominant mode of scattering.

We also notice that at low energy we find negative delay. This delay is not present exactly on the resonance but at a slightly higher energy. This effect comes from the interference between the pole λ_1 and the phase of the residue β_1. As expected, for high energy the time delay is that of the diffraction waves and the forward glory, therefore in general it is not behaving according to (4.3). The time delay oscillates with energy but it never acquires large values.

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