Another definition for time delay

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Time delay is defined by geometrical considerations which work in classical as well as in quantum mechanics, and its connection with the S matrix and the virial is proven for potentials with $V(\vec{x})$ and $\vec{x}\cdot\vec{\nabla}V(x)$ vanishing as $r^{-1-\epsilon}$ for $r\to\infty$.

INTRODUCTION

The idea of time delay as a characteristic of a scattering process was introduced by Wigner[1] and was given a precise definition by Jauch *et al.*[2] It is closely related to the existence of resonances and to the time of transit for which upper bounds are found, e.g., in Ref. 3 (although here generalized to long-range potentials).

The notion of time delay appears already in classical scattering. Here it can be defined easily by essentially geometrical considerations. Its connection with the virial and with the scattering matrix can be shown in the same way in classical and in quantum mechanics. We will not worry about domain problems although we are dealing with unbounded operators. The existence of the relevant quantities follows from estimates in Ref. 4 and references therein, if the potential $V(x)$ and $|\vec{x}\cdot\vec{\nabla}V(x)|$ decreases faster than $1/r$ and therefore its square root is H_0 and H smooth, so that the relevant quantities in the virial are integrable in time.

GEOMETRICAL CONSIDERATIONS

The existence of scattering theory implies the existence of

$$\lim_{t\to\pm\infty} p(t)=p_\pm,$$
$$\lim_{t\to\pm\infty}[x(t)-p(t)t]\equiv\lim_{t\to\pm\infty}\tilde{x}(t)=x_\pm\,. \tag{1}$$

These equations are valid for classical dynamics as well as in the quantum-mechanical problem. In the latter case the limit has to be understood as a strong limit.[5] Then $x_s=x_- - x_+$ is space delay in comparison to free time evolution. This operator has the disadvantage that it depends not only on the path but changes under time translation $t\to t+z$,

$$\{x(0),\ p(0)\}\to\{x(z),\ p(z)\},$$
$$x_\pm\to x_\pm - p_\pm z,\quad x_s\to x_s+(p_+-p_-)z\,.$$

This ambiguity can be removed if we take only the part of $x_\pm$ parallel to $p_\pm$. Then we lose the vector property and it is more natural to speak of time delay (we set $m=1$):

$$t_\pm=\frac{x_+p_\pm}{p_\pm^2}\ ,\quad \tau=\tau_- - \tau_+\,. \tag{2}$$

For notational simplicity we are concentrating on classical dynamics, although the generalization to quantum mechanics is obvious. This time delay still not only depends on the path of the particle but also on the choice of the origin in space and changes accordingly to

$$\vec{x}\to\vec{x}+\vec{a}\,,\quad \tau\to\tau-\frac{a(p_+-p_-)}{p_+^2}\,.$$

But since neither the interaction Hamiltonian nor the S matrix is invariant under space translation this ambiguity is to be expected. We shall compare now our definition of time delay with the one given in Ref. 2 (which was used in Ref. 6 for classical mechanics). Consider a sequence of balls S_R with radius R and center at $x=0$. Take τ_R to be the difference between the time a particle spends in the ball S_R if it starts at $t=-\infty$ with the same initial condition and moves either freely or accordingly to the interaction Hamiltonian. Then the limit τ_R exists and coincides with the limit of our definition. Suppose $V=0$ for $|x|>R$. If the orbit enters the ball at $t=-T_1$ and leaves it at T_2 we have

$$x_-=x(-T_1)+T_1p_-,\quad x_+=x(T_2)-T_2p_+$$

from which we obtain, as can be seen in Fig. 1, the time the particle really spends in the ball equals

$$T_1+T_2=\frac{(R^2-b^2)^{1/2}|p_+|-x_+p_+}{|p_+|^2}+\frac{(R^2-a^2)^{1/2}|p_-|+x_-p_-}{|p_-|^2}\,.$$

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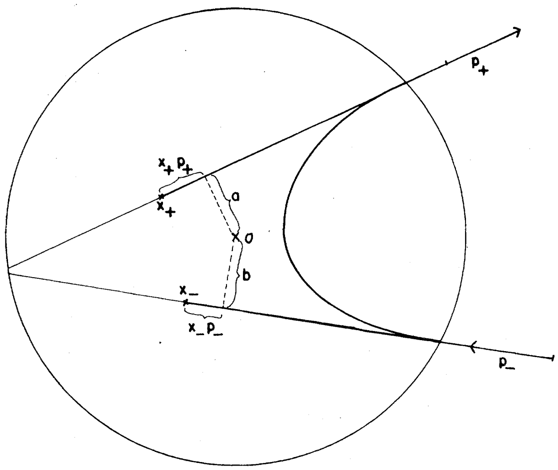

FIG. 1. Action of the scattering transformation.

A free particle would spend $2(R^2-a^2)^{1/2}/p$ and the difference becomes in the limit $R\to\infty$ equal to

$$\frac{x_-p_- - x_+p_+}{|p_+|^2} \ .$$

We can already see the connection with the S matrix which transforms x_- into x_+ (Ref. 7): For a central force S is a function $S(E,L)$. According to our considerations it corresponds for large r to a transformation

$$(r,\Phi)\to(r-p_r\,,\ \Phi')\ .$$

But as $r\to\infty$ H converges to $\frac{1}{2}p_r^{\,2}$ so we can consider $S(E,L)$ as $S(\frac{1}{2}p_r^{\,2},L)=\exp[2i\delta(p_r,L)]$. Such a transformation matrix corresponds to a transformation

$$(r,\Phi)\to\left(r-2\,\frac{\partial\delta}{p_r}\ ,\ \Phi-2\,\frac{\partial\delta}{\partial L}\right)$$

and therefore we conclude

$$\tau=\frac{2}{p_r}\,\frac{\partial\delta}{p_r}=-i\,\frac{\partial}{\partial E}\,\ln S(E,L)\ . \tag{3}$$

CONNECTION OF τ WITH THE SCATTERING MATRIX

It was shown in Refs. 8 and 9 that for potentials vanishing sufficiently at infinity (as $r^{-4-\epsilon}$) τ_R converges and becomes

$$\lim_{R\to\infty}\langle\Phi|\tau_R|\Phi\rangle = -i\left\langle\Phi_{\text{in}}\left|S^{-1}\int dE\,\delta(H_0-E)\,\frac{\partial S(E)}{\partial E}\right|\Phi_{\text{in}}\right\rangle . \tag{4}$$

Here it is understood that $\Phi=Q_{ac}\Phi$ is the state at $t=0$ corresponding to the point $\{x(0),\ p(0)\}$ in our classical consideration. Q_{ac} is the projection onto the continuous spectrum of H. S is the scattering operator in the interaction picture

$$S=\text{st-lim}\ e^{iH_0t}e^{-2iHt}e^{iH_0t}$$

and $S(E)$ is its spectral representation with respect to H_0. Φ_{in} is defined by

$$\Phi_{\text{in}}=\Omega_-^*\Phi\ ,$$

where

$$\Omega_\pm=\text{st-lim}_{t\to\pm\infty}\ e^{iHt}e^{-iH_0t}\ .$$

The proof in Ref. 6 is rather involved and the restriction for the potential is too strong. With our consideration things simplify. We will define the time delay by

$$\langle\Phi|\tau|\Phi\rangle=-\tfrac{1}{2}\lim_{t\to\infty}\left(\langle\Phi|e^{iHt}e^{-iH_0t}\overline{D}e^{iH_0t}e^{-iHt}|\Phi\rangle - \langle\Phi|e^{-iHt}e^{iH_0t}\overline{D}\,e^{-iH_0t}e^{iHt}\Phi\rangle\right)\ , \tag{5}$$

with the dilation $D=\frac{1}{2}(xp+px)$ and $\overline{D}=\frac{1}{2}[(1/H_0)D+D(1/H_0)]$. Calculating

$$\tilde{D}=e^{iHt}e^{-iH_0t}De^{iH_0t}e^{-iHt} =\tfrac{1}{2}[\tilde{x}(t)p(t)+p(t)\tilde{x}(t)]$$

with $\tilde{x}(t)$, $p(t)$ defined as in (1) we realize that our definition of time delay is defined with (2). Its connection with the S matrix remains to be proven:

$$\langle\Phi|\tau|\Phi\rangle=\tfrac{1}{2}\left[\lim_{t\to-\infty}\left\langle\Phi\left|\frac{1}{p^2(t)}\,\tilde{D}+\tilde{D}\,\frac{1}{p^2(t)}\right|\Phi\right\rangle-\lim_{t\to+\infty}\left\langle\Phi\left|\frac{1}{p^2(t)}\,\tilde{D}+\tilde{D}\,\frac{1}{p^2(t)}\right|\Phi\right\rangle\right]=\tfrac{1}{2}\langle\Phi|\Omega_-\overline{D}\Omega_-^*-\Omega_+\overline{D}\,\Omega_+^*|\Phi\rangle$$

$$=\tfrac{1}{2}\langle\Phi_{\text{in}}|\,\overline{D}-S^{-1}\overline{D}S\,|\Phi_{\text{in}}\rangle=\tfrac{1}{2}\left\langle\Phi_{\text{in}}\left|S^{-1}\,\frac{1}{H_0}[S,D]+S^{-1}[S,D]\,\frac{1}{H_0}\right|\Phi_{\text{in}}\right\rangle$$

taking into account that $[H_0, S]=0$. Now we write S in the spectral representation with respect to H_0,

$$S=\int dE\,\delta(H_0-E)S(E)$$

with $S(E)$ being a function of the angles only such that $[S(E),D]=0$. Therefore,

$$[D,S]=-i\frac{\partial}{\partial\alpha}\int dE\,\delta(\alpha^{-2}H_0-E)S(E)\Big|_{\alpha=1}$$

$$=2i\int dE\,H_0\delta(H_0-E)\frac{\partial S(E)}{\partial E}$$

and

$$\langle\Phi|\tau|\Phi\rangle=-i\left\langle\Phi_{\rm in}\left|S^{-1}\int dE\,\delta(H_0-E)\frac{\partial S(E)}{\partial E}\right|\Phi_{\rm in}\right\rangle. \tag{6}$$

It should be noted that we have to choose $\Phi\in P_{(a,\infty)}\mathcal{H}$, $a>0$, so that $\Phi_{\rm in}\in P^0_{(a,\infty)}\mathcal{H}$. Then we replace $1/p^2$ by $1/(p^2+\epsilon)$ and take finally the limit $\epsilon\to 0$.

CONNECTION WITH THE VIRIAL

The connection between time delay and the virial was already observed in Refs. 10 and 11 although here restricted to a central field and expressing the relevant terms by the phase shift and not by the S matrix. On the basis of Jauch's definition it was demonstrated by Lavine in Ref. 12. We want to prove the equivalence in our context. With D as above,

$$i\int_{-T}^{+T}dt\,\frac{1}{H}e^{iHt}[H,D]e^{-iHt}$$

$$=\frac{1}{H}(e^{iHt}De^{-iHt}-e^{-iHt}De^{iHt})$$

$$=\frac{1}{H}[p^2(T)T+p^2(-T)T+\tilde{D}(T)-\tilde{D}(-T)]\ . \tag{7}$$

On the other hand, it equals

$$-\frac{d}{d\alpha}\int_{-T}^{+T}dt\,\frac{1}{H}\,e^{iHT}e^{i\alpha D}He^{-i\alpha D}e^{-iHt}$$

$$=\int_{-T}^{+T}dt\,\frac{1}{H}(p^2-\vec{x}\cdot\vec{\nabla}V)e^{-iHt}$$

$$=4T-\int_{-T}^{+T}dt\,\frac{1}{H}e^{iHt}(2V+\vec{x}\circ\vec{\nabla}V)e^{-iHt}.$$

If we take into account that $1/p_+^2=1/p_-^2=1/2H$, and further, that our V is integrable in time and its derivative with respect to time is bounded, so that $p^2(+T)$ and $p^2(-T)$ converge to $2H$ faster than $1/T$, we can conclude

$$\tau=\lim_{T\to\infty}\tfrac{1}{2}\int_{-T}^{+T}e^{iHt}\Big[\frac{1}{H}(2V+\vec{x}\cdot\vec{\nabla}V)+(2V+\vec{x}\cdot\vec{\nabla}V)\frac{1}{H}\Big]e^{-iHt}dt. \tag{8}$$

Through this expression we see that τ exists for potentials such that V and $\vec{x}\cdot\vec{\nabla}V$ fall off like $r^{-1-\epsilon}$.

Furthermore, one can make conclusions about the sign of the time delay. Consider, e.g., a purely repulsive potential: due to repulsion the path of the particle will become shorter, due to energy conservation the velocity of the particle will become smaller and the virial tells us which effect dominates. Take $V(r)=cr^{-\nu}$. Then

$$\tau=\frac{2-\nu}{2}\int dt\left(\frac{1}{H}V+V\frac{1}{H}\right).$$

For $\nu=2$, $\tau=0$, the phase shift is independent of the energy. For $\nu<2$, $\tau<0$, the change in the velocity is the dominant effect, whereas for $\nu>2$ (where scattering theory exits for repulsive potentials) the length of the path is the relevant effect. We also see that for these potentials the phase shift is a monotonic function of the energy.

TIME DELAY FOR n PARTICLES

Based on the definition of Ref. 2 the idea of time delay was generalized to n-particle scattering theory in Ref. 13. We will sketch how this generalization can be done for our definition and leads to the same result. We ignore our insufficient knowledge about the existence and completeness of wave operators. As usual, let H_α be the channel Hamiltonians, x_α and p_α the coordinates and momenta between the clusters, and K_α the corresponding kinetic energy. Let P_α be the spectral projection operator of H_α where the corresponding individual clusters are in bound states. Define $Q_{\alpha\pm}$ to be the projection onto the range of st-lim $e^{iHt}e^{-iH_\alpha t}P_\alpha$ and assume further that our state satisfies

$$\Phi=Q_{\beta-}\Phi$$

and that

$$\Phi_{\beta\rm in}=\text{st-lim}\,e^{-iH_\beta t}e^{iHt}\Phi$$

exists. Then we define analogous to (5)

$$\langle\Phi|\tau_\beta|\Phi\rangle=\tfrac{1}{2}\lim_{t\to\infty}\left\langle\Phi\left|\sum Q_{\alpha+}e^{-iHt}e^{-iH_\alpha t}\overline{D}e^{iH_\alpha t}e^{-iHt}Q_{\alpha+}-e^{-iHt}e^{iH_\beta t}\overline{D}_\beta e^{-iH_\beta t}e^{iHt}\right|\Phi\right\rangle, \tag{9}$$

where $D_\alpha = \frac{1}{2}(x_\alpha p_\alpha + p_\alpha x_\alpha)$ and $\bar{D}_\alpha = \frac{1}{2}[(1/K_\alpha)D_\alpha + D_\alpha(1/K_\alpha)]$. Thus D_α is the dilation between the clusters and $\bar{D}_\alpha$ is the corresponding operator with the desired dimension of time. With

$$S_{\alpha\beta} = \text{st-lim} P_\alpha e^{iH_\alpha t} e^{-2iHt} e^{iH_\beta t} P_\beta ,$$

we know that

$$\sum_\alpha S^*_{\alpha\beta} S_{\alpha\beta} P_\beta = P_\beta .$$

Thus we obtain in the same way as for the one-particle case

$$\langle \Phi | \tau_\beta | \Phi \rangle = \left\langle \Phi_{\text{in}} \left| \sum_\alpha S^*_{\alpha\beta} (S_{\alpha\beta} \bar{D}_\beta - \bar{D}_\alpha S_{\alpha\beta}) \right| \Phi_{\text{in}} \right\rangle .$$

Now we know that we can write

$$S_{\alpha\beta} = \int dE\, \delta(K_\alpha - E + E_\alpha) S_{\alpha\beta}(E) = \int dE\, S_{\alpha\beta}(E)\, \delta(K_\beta - E + E_\beta) ,$$

where E_α and E_β are the energies of the clusters and $S_{\alpha\beta}$ is the unitary mapping of the $(E - E_\beta)$ shell of K_β onto the $(E - E_\alpha)$ shell of K_α. Since $\bar{D}_\alpha$ acts in the same way on K_α as $\bar{D}_\beta$ acts on K_β we obtain again by partial integration

$$\bar{D}_\alpha S_{\alpha\beta} - S_{\alpha\beta} \bar{D}_\beta = 2i \int dE\, \delta(K_\alpha - E + E_\alpha) \frac{\partial S_{\alpha\beta}(E)}{\partial E} = 2i \int dE\, \delta(H_\alpha - E) \frac{\partial S_{\alpha\beta}(E)}{\partial E}$$

and the whole time delay becomes

$$\langle \Phi | \tau_\beta | \Phi \rangle = -i \left\langle \Phi_{\text{in}} \left| \sum_\alpha S^*_{\alpha\beta} \int dE\, \delta(H_\alpha - E) \times \frac{\partial S_{\alpha\beta}(E)}{\partial E} \right| \Phi_{\text{in}} \right\rangle .$$

The virial for the n-particle case is more complicated. Its connection with the time delay can be found in an analogous way as for the one-particle problem considering

$$i \int_0^T e^{iHt} [H, \bar{D}_\alpha] e^{-iHt} dt = \bar{D}_\alpha(T) - \bar{D}_\alpha(0) = 2T + \frac{1}{2}\left[\frac{1}{K_\alpha(T)} \tilde{D}_\alpha(T) + \tilde{D}_\alpha(T) + \frac{1}{K_\alpha(T)}\right] - \bar{D}_\alpha(0) = i \int_0^T e^{iHt} [K_\alpha + I_\alpha, \bar{D}_\alpha] e^{-iHt} dt = 2T + i \int_0^T e^{iHt} [I_\alpha, \bar{D}_\alpha] e^{-iHt} dt ,$$

where I_α is the interaction between the clusters. Thus

$$\langle \Phi | \tau_\beta | \Phi \rangle = \lim_{T \to \infty} \left\langle \Phi \left| \sum_\alpha Q_{\alpha+}\, i \int_0^T dt\, e^{iHt} [\bar{D}_\alpha, I_\alpha] e^{-iHt} Q_{\alpha+} + i \int_{-T}^0 dt\, e^{iHt} [\bar{D}_\beta, I_\beta] e^{-iHt} \right| \Phi \right\rangle + \left\langle \Phi \left| \bar{D}_\beta - \sum Q_{\alpha+} \bar{D}_\alpha Q_{\alpha+} \right| \Phi \right\rangle .$$

Unfortunately results on H_α and H smoothness are missing. Also, nothing can be said about the sign of time delay essentially due to the fact that also in the one-particle case results are only available for central forces, and for many-body theory this has no meaning.

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