# Canonical scattering transformation in classical mechanics

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The quasiclassical phase shift is identified as the generator of the classical canonical $S$ transformation. This illuminates the connection between resonances and looping trajectories and the classical meaning of the time delay and Levinson's theorem. Finally the Coulomb phase shift is derived using for the time delay a free motion with a modified time dependence.

## I. INTRODUCTION

It was first recognized by Hunziker[1] that the notions of scattering theory play an important role in classical mechanics. It turned out[2] that it leads to nontrivial information for the global properties of the solutions of the classical trajectories. For instance, it shows that in the three-body problem there are large regions in phase space with $2n-1=17$ constants of motion and all trajectories in this region are homotopic to straight lines. Furthermore Wigner's[3] time delay has a simple geometrical meaning[4] for the trajectories. Recently Bollé and Osborn[5] succeeded in deriving even a classical analog to Levinson's theorem. In this paper we shall elaborate on the remark[6] that classically the phase shift corresponds to the generator of the $S$ transformation. For this purpose we define in the next section canonical coordinates for a one-, two-, and three-dimensional configuration space such that this statement assumes a simple form. This sheds some light on how trajectories with large time delays or loopings generate resonances of the quasiclassical phase shift. In the following section we give an alternative proof of the classical form of Levinson's theorem and illustrate its subtle feature by some examples. Finally we give a simple derivation of how a Dollard's[7] change in the free motion leads to the Coulomb phase shift as generator of the classical $S$ transformation for a $1/r$ potential.

We shall employ the following notations:

$$\Theta(x)\equiv\begin{cases}1 & \text{for } x>0\\ 0 & \text{for } x<0\end{cases}\quad \text{(step function)},$$

$$f\circ g(x)=f(g(x)) \quad \text{(composition of maps)},$$

$$\sup_x f(x)=\text{least upper bound of } f,$$

$$\vec{a}\times\vec{b}=\text{vector product.}$$

## II. THE $S$ TRANSFORMATION

Scattering theory investigates the asymptotic behavior of the trajectories in phase space. Although time evolution $\Phi_t$: $[x(0),p(0)]\to[x(t),p(t)]$ will not tend to a limit for $t\to\pm\infty$ it may approach another time evolution $\Phi_t^0$ such that $\Phi_{-t}\circ\Phi_t^0$ tends to a limit

$$\Omega_\pm=\lim_{t\to\pm\infty}\Phi_{-t}\circ\Phi_t^0 .$$

Since $\Phi$ and $\Phi^0$ are canonical transformations, the "Möller transformations" $\Omega_\pm$ will in general be a local canonical transformation mapping the domains $D_\pm$ into ranges $\mathcal{R}_\pm$. Closed orbits will be excluded from $\mathcal{R}_\pm$ but in reasonable[8] cases their union with $\mathcal{R}_+$ or $\mathcal{R}_-$ will fill almost all of phase space. The scattering transformation

$$S=\Omega_+^{-1}\circ\Omega_-=\lim_{t\to\infty}\Phi^0_{-t/2}\circ\Phi_t\circ\Phi^0_{-t/2}, \tag{1}$$

transforms $D_-$ into $D_+$. If $\Phi_t^0$ is the free time evolution having straight lines as trajectories, $S$ has a simple geometrical meaning. For negative $t$ $\Phi_{-t}\circ\Phi_t^0$ means that you follow the straight trajectory back for a time $-|t|$ and then continue with the actual time evolution for the same length of time. If the forces have a finite range and $\Phi$ and $\Phi^0$ coincide outside a certain region then $\Phi_{-t}\circ\Phi_t^0$ will become independent of $t$ as soon as $t$ leads you outside this region (Fig. 1). Then the limit is attained, $\Omega_-$ maps the straight line onto this trajectory of $\Phi_t$ which is asymptotically tangent to it. Similar arguments for $\Omega_+$ show that $S$ maps (Fig. 1) the straight lines tangent for $t\to-\infty$ onto the ones tangent for $t\to+\infty$. It follows from its definition that it commutes with the free time evolution: $S\circ\Phi_t^0=\Phi_t^0\circ S$. As a canonical transformation one should be able to exhibit its generator which actually is possible. We first study the special cases. The following are some examples.

### A. One-dimensional motion

Let $(x,p)$ be the canonical variables and consider the motions due to $H^0=p^2/2$, $H=p^2/2+V(x)$ where $V(x)$ has finite range or falls off sufficiently fast. The corresponding flows are

 

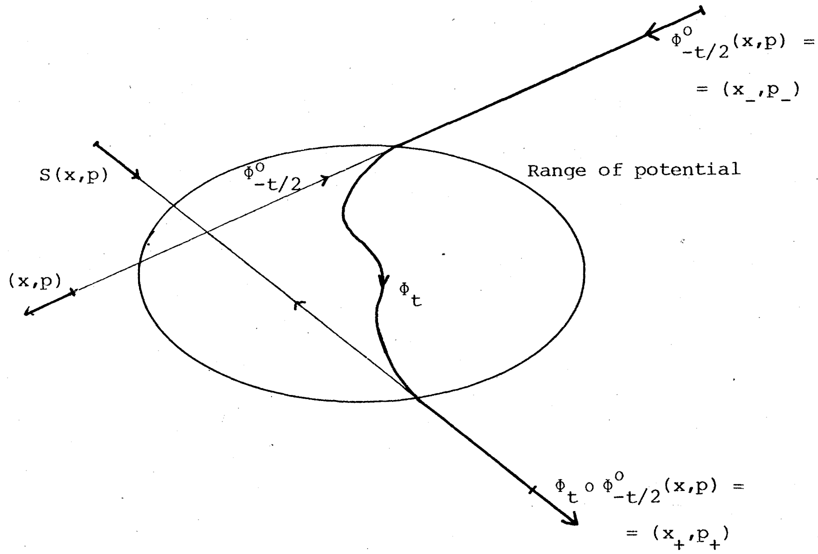


FIG. 1. Motion in configuration space.

$$\Phi^0_t:\ (x,p)\rightarrow(x+pt,p),\qquad(2)$$
$$\Phi_t(x,p)\rightarrow[x(t),\{p^2+2[V(x)-V(x(t))]\}^{1/2}].$$

If $p^2>\sup_x 2V(x)$, so that there is no reflection, $x(t)$ is determined by

$$t=\int_x^{x(t)}\frac{d\alpha}{\{p^2+2[V(x)-V(\alpha)]\}^{1/2}}.$$

In this case the $S$ transformation can be easily constructed. If we call

$$x_-=\Phi^0_{-t/2}(x)=x-pt/2,\quad x_+=\Phi_t(x_-),$$

then

$$\Phi^0_{-t/2}\circ\Phi_t\circ\Phi^0_{-t/2}$$

acts as

$$(x,p)\xrightarrow{\Phi^0_{-t/2}}(x-pt/2,p)\xrightarrow{\Phi_t}\left(x-pt/2+\int_{x_-}^{x_+}d\alpha,[p^2+2V(x_-)-2V(x_+)]^{1/2}\right)$$
$$\xrightarrow{\Phi^0_{-t/2}}\left(x-\frac{t}{2}\left(p+[p^2+2V(x_-)-2V(x_+)]^{1/2}\right)+\int_x^{x_+}d\alpha,[p^2+2V(x_-)-2V(x_+)]^{1/2}\right),\qquad(3)$$

where

$$t=\int_{x_-}^{x_+}\frac{d\alpha}{\{p^2+2[V(x_-)-V(\alpha)]\}^{1/2}}.$$

For $t\rightarrow\infty$ we have $x_-\rightarrow-\infty$, $x_+\rightarrow+\infty$, and $V(x_-)$, $V(x_+)\rightarrow0$. Then

$$(x,p)\xrightarrow{S}\left(x-p\int_{-\infty}^{\infty}d\alpha\left(\frac{1}{[p^2-2V(\alpha)]^{1/2}}-\frac{1}{(p^2)^{1/2}}\right),p\right)\equiv(x-p\tau,p),\qquad(4)$$

i.e., $S$ changes $x$ by $p$ times the time delay $\tau$. The latter is the difference of the times the actual and the free time evolutions need for the trajectory from $(x_-,p_-)$ to $(x_+,p_+)$ in the limit $x_-\rightarrow-\infty$, $x_+\rightarrow+\infty$ (Fig. 2). $S$ is the canonical transformation $(x,p)\rightarrow(x-2\partial\delta(p)/\partial p,p)$ where

$$\delta(p)=\tfrac{1}{2}\int_{-\infty}^{\infty}d\alpha\{[p^2-2V(\alpha)]^{1/2}-(p^2)^{1/2}\}.$$

If there is an $x_1$ such that $p^2<2V(x_1)$ then a trajectory with $x<x_1$, $p>0$ will be reflected to the left. In this

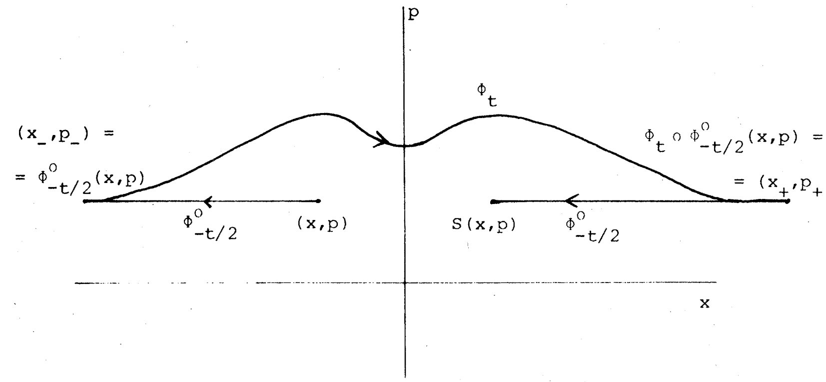


FIG. 2. One-dimensional motion in phase space.

case the action (3) of $S$ is changed to $[V_- \equiv V(x_-)$, etc.]

$$(x,p) \xrightarrow{\Phi^0_{-t/2}} (x-pt/2,p) \xrightarrow{\Phi_t} (x_+,\ -(p^2+2V_--2V_+)^{1/2}) \xrightarrow{\Phi^0_{-t/2}} \left(x_+ + \frac{t}{2}(p^2+2V_--2V_+)^{1/2},\ -(p^2+2V_--2V_+)^{1/2}\right).$$

Here

$$t = \int_{x_-}^{x_0} \frac{d\alpha}{[p^2+2V_--2V(\alpha)]^{1/2}} + \int_{x_+}^{x_0} \frac{d\alpha}{[p^2+2V_--2V(\alpha)]^{1/2}},$$

where the reflection point $x_0$ is the smallest $x$ with $2V(x)=p^2+2V_-$. If $x_0<0$ we may write

$$x_+ = -x_- - \int_{x_+}^{x_0} d\alpha - \int_{x_0}^{-x_0} d\alpha - \int_{-x_0}^{-x_-} d\alpha,$$

and thus for $t\to\infty$ we obtain

$$(x,p) \xrightarrow{S} \left(\lim_{t\to\infty}\left(-x+pt/2 - \int_{x_+}^{x_0} d\alpha - \int_{x_0}^{-x_0} d\alpha - \int_{-x_0}^{-x_-} d\alpha + \frac{t}{2}(p^2+2V_--2V_+)^{1/2},\ -(p^2+2V_--2V_t)^{1/2}\right)\right)$$

$$= \left(-x + 2p\int_{-\infty}^{x_0} d\alpha\left(\frac{1}{[p^2-2V(\alpha)]^{1/2}} - \frac{1}{(p^2)^{1/2}}\right) - \int_{x_0}^{-x_0} d\alpha,\ -p\right).$$

Thus the time delay is in comparison with a free motion going up to the origin. If $V$ is twice differentiable it becomes infinite when $p^2$ approaches $2\sup_x V(x) = 2V(x_0)$ because

$$\int \frac{d\alpha}{[V''(x_0-\alpha)^2]^{1/2}} = \infty.$$

Then there is an orbit which approaches $x_0$ for $t\to\infty$ and for this value of $p$ $S$ does not exist. It separates the region in phase space where $S$ is of the form (3) and the present case (Fig. 3) where

$$(x,p) \xrightarrow{S} \left(-x + 2\frac{\partial\delta(p)}{2p},\ -p\right),$$

$$\delta(p) = \int_{-\infty}^{x_0(p)} d\alpha\{[p^2-2V(x)]^{1/2} - p\,|x_0(p)|\,.$$

For example, the square-well potential $V(x) = V\Theta(R-|x|)$ gives

$$\delta(p) = \begin{cases} R((p^2+2|V|)^{1/2} - (p^2)^{1/2}) & \text{for } V<0 \\ = \begin{cases} R((p^2-2V)^{1/2} - p^2) & \text{if } p^2>2V \\ -pR \quad \text{if } p^2<2V \end{cases} & \text{for } V>0\,. \end{cases}$$

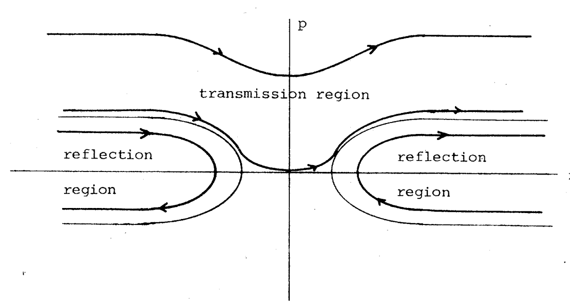


FIG. 3. Trajectories in phase space for a repulsive potential.

### B. Two-dimensional motion

Consider again $H^0=\vec{p}^2/2$, $H=\vec{p}^2/2+V(x)$. It is convenient to use the variables $p=|\vec{p}|$, $a=\vec{p}\cdot\vec{x}/p$, $L=|\vec{x}\times\vec{p}|$, and $\chi=\arccos p_x/p$, i.e. (Fig. 4),

$$p_x=p\cos\chi,\quad x=a\cos\chi-\frac{L}{p}\sin\chi\,,$$

$$p_y=p\sin\chi,\quad y=a\sin\chi+\frac{L}{p}\cos\chi\,.$$

Since $L$ generates a rotation and $(\vec{p}\cdot\vec{x})$ the dilation $(x,p)\to(xe^{\beta},pe^{-\beta})$ one sees readily that the new variables are canonical, i.e., $\{a,p\}=\{\chi,L\}=1$, the other Poisson brackets vanishing. The free time evolution is simply $(a,\chi;p,L)\to(a+pt,\chi,p,L)$ but in general $\phi_t$ will be complicated. $S$ maps free trajectories into free trajectories and will be of the form

$$(a,\chi;p,L)\xrightarrow{S}(a-p\tau,\chi';p,L')\,,$$

$\chi'$ and $L'$ independent of $a$. If $V$ is a central potential $V(|\vec{x}|)$ or more generally of the form $V(|\vec{x}|,L)$ so that $L$ is constant, then $\Phi_t$ can be reduced to a one-dimensional problem and $S$ constructed explicitly. The chain (3) of maps becomes in that notation

$$(a,\chi;p,L)\xrightarrow{\Phi^0_{-t/2}}(a-pt/2,\chi,p,L)\xrightarrow{\Phi_t}\left(a-pt/2+\int_{a_-}^{a_+}da,\chi';[p^2+2(V_--V_+)]^{1/2},L\right)$$

$$\xrightarrow{\Phi^0_{-t/2}}\left(a-\frac{t}{2}(p+[p^2+2(V_--V_+)]^{1/2}+\int_{a_-}^{a_+}+d\alpha,\chi',[p^2+2(V_--V_+)]^{1/2},L\right).\tag{5}$$

Again for $t\to\infty$ we have $|a_+|$, $|a_-|\to\infty$, $V_+$, and $V_-\to 0$. The time $t$ for the actual motion $\Phi_t$ is readily expressed as integral over $r\equiv|\vec{x}|=(a^2+L^2/p^2)^{1/2}$ with $E=p^2/2+V_-$,

$$t=\int_{r_0}^{r_-}\frac{dr}{[2E-L^2/r^2-2V(r)]^{1/2}}+\int_{r_0}^{r_+}\frac{dr}{[2E-L^2/r^2-2V(r)]^{1/2}}\,,$$

where $\sqrt{\phantom{x}}=O$ for $r=r_0$. Since $a=(r^2-L^2/p^2)^{1/2}=r+O(1/r)$ and $da=p\,dr/(p^2-L^2/r^2)^{1/2}$ we have for $r_+,r_-\to\infty$:

$$\int_{a_-}^{a_+}d\alpha=\left(\int_{L/p}^{r_-}+\int_{L/p}^{r_+}\right)\frac{p\,dr}{(p^2-L^2/r^2)^{1/2}}\,.$$

Thus in the limit $t\to\infty$ we arrive at

$$(a,\chi;p,L)\xrightarrow{S}\left(a-2\frac{\partial\delta(p,L)}{\partial p},\chi-2\frac{\partial\delta(p,L)}{\partial L},p,L\right),$$

$$\delta(p,L)=\lim_{R\to\infty}\left(\int_{r_0}^{R}dr[p^2-L^2/r^2-2V(r)]^{1/2}-\int_{L/p}^{R}dr(p^2-L^2/r^2)^{1/2}\right).\tag{6}$$

Here we have used the well-known expression for the scattering angle $\chi-\chi'$. Let us consider the two-dimensional $S$ transformation for typical potentials.

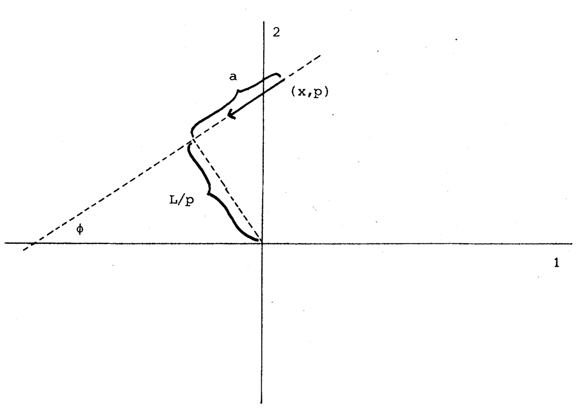


FIG. 4. The canonical coordinates in two dimensions.

#### 1. $1/r^2$ potential

If $V(r)=c/r^2$ then $S$ exists only for $c>-L^2/2$. In the attractive case trajectories with the impact parameter, and therefore $L$ too small, spiral into the origin. For the others the $r$ integral is easily calculated, for instance, by complex integration. Evaluating the residue at the origin we find

$$\delta(p,L)=\frac{\pi}{2}[(L^2+2c)^{1/2}-L]\,.$$

Since $\delta$ is independent of $p$ the time delay is zero. This is related to the dilation properties of the Hamiltonian [compare Ref. 2(a), Sec. 3.4.15.3]. The scattering angle $\pi[L/(L^2+2c)^{1/2}-1]$ tends to $\infty$ for $c<0$ for those $L$ where spiral orbits set in.

#### 2. Square-well potential

If $V(r)=c\Theta(R-r)$ we find

$$\delta(p,L)=\left([(p^2-2c)R^2-L^2]^{1/2}+L\arcsin\frac{L}{R(p^2-2c)^{1/2}}\right)\Theta(p^2R^2-L^2)\Theta((p^2-2c)R^2-L^2)$$
$$-\left((p^2R^2-L^2)^{1/2}+L\arcsin\frac{L}{Rp}\right)\Theta(p^2R^2-L^2).$$

In the attractive case $\delta$ is discontinuous for $p^2=2c+L^2/R^2$ because there $r_0$ jumps from $L/(p^2-2c)^{1/2}$ to $L/p$ (see Fig. 5).

Thus $\delta$ is given in the two regions $p^2 \lessgtr 2c+L^2/R^2$ by different expressions whereas on the separating hypersurface $S$ does not exist. For a rounded-off potential there are the trajectories which asymptotically reach the maximum of the potential but never get over it. For a twice differentiable potential the time delay would become $\infty$ whereas for the square well

$$\tau=\frac{2}{p}\frac{\partial\delta}{\partial p}=\frac{2}{p^2}[(p^2R^2-L^2-2cR^2)^{1/2}-(p^2R^2-L^2)^{1/2}]$$

remains finite. In any case this is the closest similarity to a quantum mechanical resonance since the special value $\delta/\hbar=\pi/2$ has classically no significance.

### C. Three-dimensional motion

There are many canonical coordinate systems such that the free motion just shifts one coordinate. We shall choose one where $|\vec{p}|$, $L$, and $L_z$ occur such that for central potentials the $S$ transformation is simple. A convenient choice are the coordinates used in [Ref. 2(a), Sec. 5.3.4] with $\vec{x}$ and $\vec{p}$ exchanged (see Fig. 6)

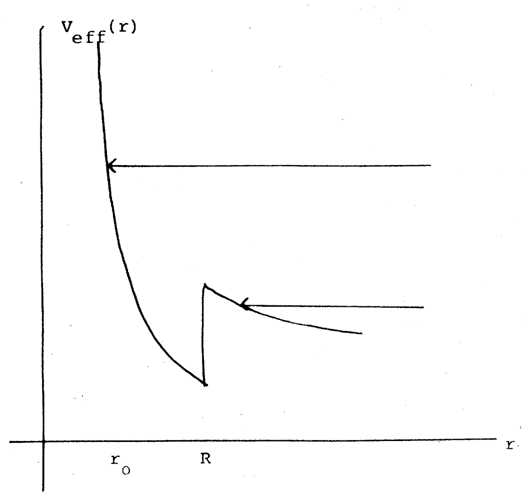


FIG. 5. The effective square-well potential.

$$p=(p_x^2+p_y^2+p_z^2)^{1/2}, \quad L=|\vec{x}\times\vec{p}|, \quad L_z=[x\times p]_z,$$
$$a=\frac{\vec{x}\cdot\vec{p}}{p}, \quad \chi=\arc\cos\frac{L_xp_y-L_yp_x}{p(L_x^2+L_y^2)^{1/2}},$$
$$\phi=\arc\cos\frac{L_y}{(L_x^2+L_y^2)^{1/2}}.$$

$\chi$ is the angle of momentum in the plane of motion and $\phi$ is the angle of the projection of $\vec{L}$ in the $(x,y)$ plane. For the proof of the canonicity of these coordinates, see (2). The free motion is $(a,\chi,\phi;p,L,L_z)\to(a+pt,\chi,\phi;p,L,L_z)$. For a central potential the trajectory remains in a plane and the $S$ transformation can be found as in $b$

$$(a,\chi,\phi;p,L,L_z)\to\left(a-2\frac{\partial\delta(p,L)}{\partial p},\chi-2\frac{\partial\delta(p,L)}{\partial L},\right.$$
$$\left.\phi;p,L,L_z\right),$$

$$\delta(p,L)=\lim_{R\to\infty}\left(\int_{r_0}^{R}dr[p^2-L^2/r^2-2V(r)]^{1/2}\right.$$
$$\left.-\int_{r_0'}^{R}dr(p^2-L^2/r^2)^{1/2}\right).$$

#### 1. Remarks

(1) We see that the generator of $S$ is the so-called[8] quasiclassical approximation for the quantum-mechanical phase shift $\delta/\hbar$. A close relation is to be expected since the quantum-mechanical $S$ matrix $S=e^{2i\delta/\hbar}$ generates the above transformation. However, the expression (6) is classically not an uncontrollable approximation but the exact result.[9]

(2) The limit $R\to\infty$ exists if $V$ decreases for $r\to\infty$ as $r^{-1-\epsilon}$, $\epsilon>0$. In this case one sees easily that also the limit $t\to\infty$ in the definition of $S$ exists.

(3) In the two- and three-dimensional case the time delay is measured by comparing the time of the trajectory with the following free motions: Follow the one tangent for $t\to-\infty$ up to $r_0'$, i.e., the point of closest approach to the origin, then switch over to the free trajectory tangent for $t\to+\infty$ at the same $r_0'$.

(4) Since $pa=(xp)$ generates dilations its change under $S$ is given by a generalization of the virial theorem to infinite trajectories. One finds for the time delay[4]

$$\tau=\frac{1}{E}\int_{-\infty}^{\infty}dt[2V(x(t))+\vec{x}(t)\vec{\nabla}V(x(t))].$$

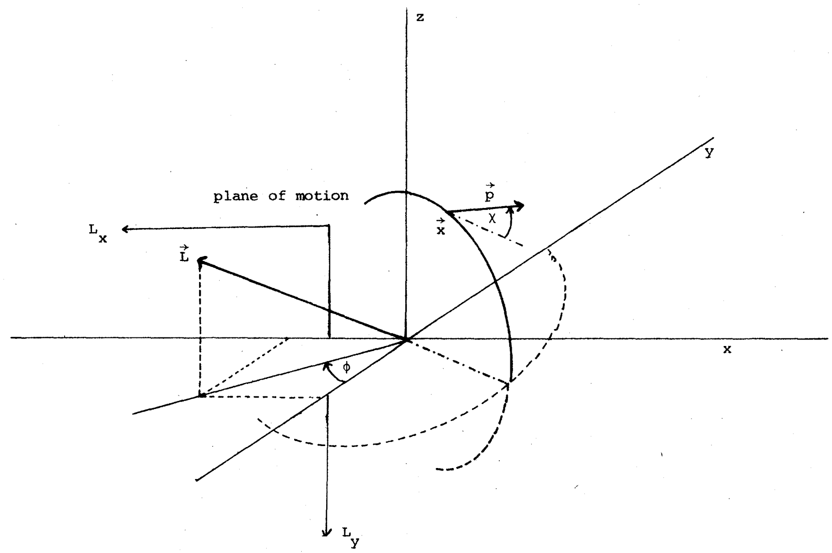


FIG. 6. The canonical coordinates in three dimensions.

(5) Since $\delta(p,L)$ goes to zero for $L\to\infty$ we may write

$$\delta(p,L)=\tfrac{1}{2}\int_L^\infty dL'[\chi'(p,L,\chi)-\chi]\,.$$

$\delta$ has the dimension of an action. Choosing $\hbar$ as a unit of angular momentum,

$$\frac{1}{\hbar}\delta=\tfrac{1}{2}\int\frac{dL'}{\hbar}(\ )$$

becomes dimensionless. If the deflection angle exceeds $\pi$ over an interval $\hbar$ and otherwise keeps the same sign the $\delta/\hbar$ goes beyond 90°. Thus we see the following connection between resonances and looping trajectories. A looping for all angular momenta in the interval $(L',L'+\hbar)$ and $L'>L$ implies a "resonance" in the sense that the quasi-classical $\delta(p,L)$ is larger than 90°. Generally resonances occur for those $L$ for which the sum of the deflection angles for larger $L$'s reaches 180°. An analogous statement can be made with respect to the time delay since

$$\delta(p,L)=\int_p^\infty p'dp'\tau(p',L)\,.$$

(6) If $H=H^0+\lambda V$ we see

$$\frac{\partial\delta}{\delta\lambda}=-\tfrac{1}{2}\int_{-\infty}^{\infty}dt\,V(x(t))\,.$$

This is the classical version of an analog to the Hellmann-Feynman formula in scattering theory.[10] Thus also classically $V\gtrless 0$ implies $\delta\lessgtr 0$. If we were to confine the system in a ball with radius $R$ the right-hand side above is $-R/p\cdot$(time average of $V$). This is a classical analog of Schwinger's relation between phase shift and energy shift of the system in ball. This furthermore shows that Kato's monotonicity[13] is classically obvious.

(7) Although we don't have a general explicit expression for $\Omega_\pm$ outside the range of the potential for a $>0\Omega_+$ is 1 and $\Omega_-$ therefore equals $S$. Similarly for a $>$ o $\Omega_-=\Pi$ and $\Omega_+=S^{-1}$.

(8) Everybody conversant with modern classical mechanics has more powerful methods available than the pedestrian ones employed so far. They would generalize our results as follows. Since the time evolution changes the canonical 1 form by the exterior derivative of the action [see Refs. 1 and 2(a), Sec. 3.2.9] we have with the previous notation

$$\vec{p}_-\cdot d\vec{q}_-=\vec{p}\cdot d\vec{q}+dw_-^0\,,\quad (q_+,p_-)=\Phi^0_{-t/2}(q,p)\,,$$

$$w_-^0=-\int_{-t/2}^{0}dt'\,\Phi^0_{t'}\left(\frac{\vec{p}^2}{2}\right)\,,$$

$$\vec{p}_+\cdot d\vec{q}_+=\vec{p}_-\cdot d\vec{q}_-+dw\,,\quad (q_+,p_+)=\Phi_t(q_-,p_-)\,,$$

$$w=\int_0^t dt'\,\Phi^0_{t'}\left(\frac{\vec{p}_-^2}{2}-V(x_-)\right)\,,$$

$$\vec{p}_s\cdot d\vec{q}_s=\vec{p}_+\cdot d\vec{q}_++dw_+^0\,,\quad (q_s,p_s)=\Phi^0_{-t/2}(q_+,p_+)\,,$$

$$w_t^0=-\int_{-t/2}^{0}dt'\,\Phi^0_{t'}\left(\frac{\vec{p}_+^2}{2}\right)\,.$$

Adding these equations up gives

$$\vec{p}_s\cdot d\vec{q}_s=\vec{p}\cdot d\vec{q}+d(w+w_-^0+w_+^0)$$

and thus for $t\to\infty$ the general form of the generator of $S$: $(q,p)\to(q_s,p_s)$. For the evaluation of the path integrals one may use

$$\int_0^t dt'\Phi_{t'}\left(\frac{p^2}{2}-V(q)\right)$$
$$=\int_q^{q_t} dq'[p^2+2V(q)-2V(q')]^{1/2}-Et\,,$$

and rederive the previous expressions. Jajima[12] has shown that the difference between the action and the free action is the classical limit of the quantum phase shift. To make it useful as generator of a classical canonical transformation is a matter of finding the appropriate canonical variables.

## III. THE CLASSICAL LEVINSON THEOREM

Levinson's theorem relates the change of the phase between $E=0$ and $E=\infty$ to the number of bound states. This seemingly wave-mechanical statement corresponds to a classical geometrical fact relating the volume in phase space of the bound orbits to the integral over the time delay. We shall now give a simple derivation of this relation using the fact that $\Omega$ and $S$ as canonical transformation preserve the volume in phase space.

Let the phase space be decomposed by the characteristic functions $\chi_b$ and $\chi_s$ into the regions of bound orbits and scattering trajectories. $\chi_b$ is 1 in the former and 0 in the latter region and $\chi_s$ vice versa. Furthermore we first confine the integration to compact regions in phase space by the characteristic function

$$\Theta_E(x,p)=\begin{cases}1 & \text{if } \mathrm{H}(x,p)<E\\ 0 & \text{otherwise}\end{cases}$$
$$\Theta_R(x,p)=\begin{cases}1 & \text{if } x^2<R^2\\ 0 & \text{otherwise}.\end{cases} \tag{7}$$

Now

$$\int d^\nu x d^\nu p\Theta_E\Theta_R=\int d^\nu x\, d^\nu p\,\Theta_E\Theta_R(\chi_b+\chi_s)$$
$$=\int d^\nu x\, d^\nu p\,\Theta_E\Theta_R\chi_s$$
$$+\int d^\nu x\, d^\nu p\,\Theta_E\circ\Omega_+\Theta_R\circ\Omega_+ \tag{8}$$

since $\chi_s\circ\Omega_+$ is one. Furthermore $\Theta_E\circ\Omega_+ =\Theta(E-p^2/2)$ such that

$$\int d^\nu x\, d^\nu p\,\Theta_E\Theta_R\chi_b=\int d^\nu x\, d^\nu p\,\Theta_R(\Theta_E-\Theta(E-p^2/2))$$
$$+\int d^\nu x\, d^\nu p\,\Theta(E-p^2/2)(\Theta_R-\Theta_R\circ\Omega_+)\,. \tag{9}$$

We now have to consider the limits $R\to\infty$, $E\to\infty$ and assume that the potential is reasonable enough so that this can be done with impunity. For the discussion of the right-hand side we distinguish between different dimensions.

### A. $\nu=1$

Assume that $V(x)$ is uniformly bounded $c_1\leq V(x)\leq c_2$. Then

$$\lim_{R\to\infty}\int dx\,dp\,\Theta(R^2-x^2)\times\left[\Theta\left(E-\frac{p^2}{2}-V(x)\right)-\Theta\left(E-\frac{p^2}{2}\right)\right]$$
$$=\int dx\, 2(\{2[E-V(x)]\}^{1/2}-\sqrt{2E}),\quad \text{for } E>c_2\,. \tag{10}$$

This integral exists if $V$ is integrable (which is necessary for the existence of scattering theory) and tends to zero for $E\to\infty$ as $(2/\sqrt{2E})\int dx\,V(x)$. For discussing the last term we assume first that the potential has finite support such that $V(x)=0$ for $|x|>R_0$. Then according to remark (7) in Sec. II,

$$\chi_R\circ\Omega_+=\Theta(xp)\Theta_R+\Theta(-xp)\Theta_R\circ S^{-1}\,. \tag{11}$$

If the potential does not have finite support but decreases faster than $1/|x|^{1+\epsilon}$ then (11) can be replaced by

$$\lim_{R\to\infty}[\Theta_R\circ\Omega_+-\Theta(xp)\Theta_R-\Theta(-xp)\Theta_R\circ S^{-1}]=0\,. \tag{12}$$

The effect of $S^{-1}$ on $x$ is known to be the shift $p\tau(p)$. The last term contributes only for $xp<0$ and then only if an $|x|<R$ is shifted by $S$ to be $>R$ or vice versa. Thus the $x$ integral picks up $p\tau$ from one end or the other.

$$\lim_{R\to\infty}\int dx\,dp\,\Theta\left(E-\frac{p^2}{2}\right)(\Theta_R-\Theta_R\circ\Omega_+)$$
$$=-\int dp\,|p|\tau(p)\Theta\left(E-\frac{p^2}{2}\right)$$
$$=-2\int d\epsilon\,\tau(\epsilon)\Theta(E-\epsilon)\,.$$

Thus finally in the limit $E\to\infty$ we arrive at

$$\int dx\,dp\,\chi_b=-\int dp\,|p|\tau(p)\,. \tag{13}$$

#### *Examples*

(1) If $V(x)<0$ then

$$\int dx\,dp\,\chi_b=\int dx\,dp\,\Theta(2|V(x)|-p^2)$$
$$=\int dx\,2[2|V(x)|]^{1/2}\,.$$

On the other hand

$$-\int dp\,|p|\,\tau(p) = -\int dx \times \int |p|\,dp\left(\frac{1}{[p^2-2V(x)]^{1/2}} - \frac{1}{(p^2)^{1/2}}\right) = 2\int dx[2|V(x)|]^{1/2}.$$

(2) Repulsive square well $\chi_b = 0$. According to Sec. II we have

$$\tau = 2R\begin{cases}\dfrac{1}{(p^2-2V)^{1/2}} - \dfrac{1}{(p^2)^{1/2}} & \text{for } p^2 > 2V\\[2mm] -\dfrac{1}{|p|} & \text{for } p^2 < 2V\end{cases}$$

and in fact

$$\int_0^\infty dp\,p\tau(p) = \int_0^{\sqrt{2V}} dp(-2R) + \int_{(2V)^{1/2}}^\infty dp\,2R\left(\frac{1}{(p^2-2V)^{1/2}} - \frac{1}{(p^2)^{1/2}}\right) = 0.$$

### B. $\nu = 2$

For $E > c_2$ the first term in (9) becomes simple and $E$ independent

$$\int d^2x\,d^2p\left[\Theta\left(E - \frac{p^2}{2} - V(x)\right) - \Theta\left(E - \frac{p^2}{2}\right)\right] = -2\pi\int d^2x\,V(x).$$

For calculating the last integral (11) remains valid for potentials with compact support. The statement (12) becomes too weak for two dimensions, because the $x$ integration runs over a sphere and there it has to be replaced by the condition

$$\lim_{R\to\infty} R^{1+\epsilon}[\Theta_R\circ\Omega_+ - \Theta_R\circ S^{-1}\Theta(-xp) - \Theta_R\Theta(xp)] = 0. \qquad (12')$$

This condition is met by potentials decreasing faster than $1/r^{2+\epsilon}$.

Fixing $\vec{p}$ the integration over $x$ runs over half of the sphere after replacing $\Omega$ by $S^{-1}$. The time delay depends on $p$ and $L$ and $\phi$ (which we can forget after fixing $\vec{p}$). Since we already assumed that $V$ vanishes sufficiently at infinity it follows that

$$\lim_{L\to\infty} L^{1+\delta}\tau(p,L,\phi) = 0,$$

so that $\tau$ is integrable in $L$. Now we turn to the coordinates introduced in Sec. II for $\nu = 2$. Since $|\vec{x}| = a + 0(1/a)$ the action of $S$ for large $|\vec{x}|$ becomes $S(|\vec{x}|) = S(|\vec{x}| - p\tau)$. Thus for $R\to\infty$, $\Theta_R - \Theta_R\circ S^{-1}$ becomes $\Theta(R - |\vec{x}|) - \Theta(R - |\vec{x}| - p\tau)$. Since the coordinates are canonical the volume element in phase space is $dp\,da\,dL\,d\phi$ and the integral can be treated as for $\nu = 1$. We find

$$\lim_{R\to\infty}\int d^2x\,d^2p(\Theta_R - \Theta_R\circ S^{-1})\Theta(-xp)\Theta\left(E - \frac{p^2}{2}\right) = -\int dp\,d\phi\,\Theta\left(E - \frac{p^2}{2}\right)dL\,p\tau(p,L,\phi),$$

or in the case of a spherical symmetric potential,

$$= -2\pi\int d\epsilon\,\Theta(E-\epsilon)dL\,\tau(\epsilon,L).$$

It should be noted that for $E > c_2$ the first and second expressions in (9) become $E$ independent, thus it follows that for $E > c_2$ we must have

$$\int dL\,d\phi\,\tau(p,L,\phi) \equiv 0.$$

For spherical symmetric potentials this can be shown explicitly

$$\tau(\epsilon,L) = 2\int dr\left(\frac{1}{\{2[\epsilon - V(r)] - L^2/r^2\}^{1/2}}\Theta(r - r_0(L,p)) - \frac{1}{(2\epsilon - L^2/r^2)^{1/2}}\Theta(r - L/p)\right),$$

where $V(r_0) + L^2/2r_0^2 = \epsilon$. Thus after changing the order of integration the two contributions cancel upon $L$ integration:

$$\int dr\,r\left(\int_0^{r\{2[\epsilon - V(r)]\}^{1/2}} \frac{dL}{\{2[\epsilon - V(r)]r^2 - L^2\}^{1/2}} - \int_0^{r(2\epsilon)^{1/2}} \frac{dL}{(2\epsilon r^2 - L^2)^{1/2}}\right) = 0.$$

Thus in two dimensions Levinson's theorem reads

$$\int d^2p\,d^2x\,\chi_b = -2\pi\int d^2x\,V(x) - \int d^2p\,dL\,\tau(\vec{p},L).$$

We note a correction term which has already been found in Ref. 5.

### C. $\nu = 3$

The first term on the rhs of (9) now becomes (again for $E > c_2$)

$$\int d^3x\,d^3p\left[\Theta\left(E - \frac{p^2}{2} - V(x)\right) - \Theta\left(E - \frac{p^2}{2}\right)\right] = \frac{4\pi}{3}2^{3/2}\int d^3x\{[E - V(x)]^{3/2} - (E)^{3/2}\},$$

which in leading order in $E$

$$= -4\pi \int d^3x\,(2E)^{1/2} V(x)\,.$$

The evaluation of the last term is completely analogous as for two dimensions. The condition on the potential has to be strengthened to $V(r)$ decreases as $1/r^{3+\epsilon}$. Thus

$$\lim_{R\to\infty} R^{2+\epsilon}[\Theta \circ \Omega_+ - \Theta_R \circ S^{-1}\Theta(-xp) - \Theta_R\Theta(xp)] = 0$$

suffices for replacing $\Omega$ by $S$. The integration over the surface of the half-ball can be replaced in the limit $R\to\infty$ by that over the half-phase such that we obtain

$$\lim_{R\to\infty} \int d^3x\, d^3p\,(\Theta_R - \Theta_R \circ S^{-1})\,\Theta(-xp)\Theta\left(E - \frac{p^2}{2}\right) = - \int dp\, d\phi\, d\chi\, \Theta\left(E - \frac{p^2}{2}\right) dL\, dL_z\, p\tau(p, L, L_z, \phi, \chi)\,.$$

Generally the result for $\nu = 3$ is

$$\int d^3p\, d^3x\, \chi_b = \lim_{E\to\infty}\left(-(2E)^{1/2} 4\pi \int d^3x\, V(x) - \int_0^{(2E)^{1/2}} dp \int d\phi\, d\chi\, dL_z\, dL\, p\tau\right).$$

Since the left-hand side of (9) becomes independent of $E$ for sufficiently large $E$ we obtain the relation

$$\int d\phi\, d\chi\, dL_z\, dL\, \tau = 4\pi \int d^3x \{2[E - V(x)]^{1/2} - (2E)\}^{1/2}, \quad VE > \sup_x V(x)\,.$$

For a spherical potential this relation can be checked explicitely since

$$\int d\phi\, d\chi\, dL_z\, dL\, \tau(p, L) = 4\pi^2 \int_0^{L_{\max}} dL^2 2 \int dr \left(\frac{1}{\{2[E - V(r)] - L^2/r^2\}^{1/2}} - \frac{1}{(2E - L^2/r^2)^{1/2}}\right)$$

$$= 16\pi^2 \int r^2 dr \{2[E - V(r)]^{1/2} - (2E)\}^{1/2}\,.$$

It should be noted that in more than 1 dimension a negative potential does not necessarily generate a negative time delay. Though the particle becomes faster it may have to cover a longer trajectory.

## IV. THE COULOMB POTENTIAL

For $V = (e^2/r)\lim_{t\to\infty}\Phi_t \circ \Phi^0_{-t}$ does not exist: $\Phi^0_{-t}$ maps $\vec{x}$ into $\vec{x}-\vec{p}t$ but for the Kepler motion this quantity goes for $t\to\infty$ as $10nt$. Following Dollard[7] one considers another $\Phi^0_t$ which has also straight trajectories but covered with a nonuniform speed. In the notation of Sec. II in two and three dimensions the free motion $\Phi^0_{-t}$ is

$$a \to a - pt - \frac{e^2}{p^2}\ln(t+1)\frac{p}{2}\,,$$

the other variables remaining constant. Then the chain of maps (5) changes $a$ (for $t\to\infty$) into

$$a - pt - \frac{2e^2}{p^2}\ln\frac{tp}{4} + \int_{a_-}^{a_+} d\alpha\,,$$

where

$$t/2 = \int_{r_0}^{R} \frac{dr}{\left(p^2 - \frac{2e^2}{r} - \frac{L^2}{r^2}\right)^{1/2}} = \frac{1}{p}\left[\left(R - \frac{e^2}{p^2}\right)^2 - \frac{L^2}{p^2} - \frac{e^4}{p^4}\right]^{1/2}$$

$$+ \frac{e^2}{p^3}\,\mathrm{arcosh}\frac{R - e^2/p^2}{\left(\frac{L^2}{p^2} + \frac{e^2}{p^4}\right)^{1/2}} \overset{R\to\infty}{\simeq} \frac{R}{p} - \frac{e^2}{p^3} + \frac{e^2 \ln R}{p^3} - \frac{e^2}{2p^3}\ln\left(L^2 + \frac{e^4}{p^2}\right) + \frac{e^2}{p^3}\ln\frac{p}{2}\,,$$

and $a_{\pm}=R+O(1/R)$. Thus for $R\to\infty$ we find

$$S(\mathrm{a})=a+\frac{2e^2}{p^2}+\frac{e^2}{p^2}\ln\left(L^2+\frac{e^4}{p^2}\right).$$

Using the well-known expression for the Coulomb scattering angle we have in three dimension,

$$S(a,\chi,\phi,p,L,L_z)\to\left(a-2\frac{\partial\delta(p,L)}{p},\ -2\frac{\partial\delta(p,L)}{L},\ \phi;\ p,L,L_z\right)$$

$$\delta(p,L)=\frac{1}{2i}\left[\left(L+\frac{ie^2}{p}\right)\ln\left(L+\frac{ie^2}{p}\right)-\left(L-\frac{ie^2}{p}\right)\ln\left(L-\frac{ie^2}{p}\right)\right].$$

### *Remarks*

(1) $\Phi_t^0$ is for fixed $t$ a canonical transformation but $\Phi^0$ is not a one parameter group. Its choice is to a large extent arbitrary, one has only to see that the $\ln R$ term cancels. This liberty affects the time delay but not the scattering angle.

(2) It is remarkable that for the smooth potentials $V=1/r$ or $1/r^2$ the classical and quantum $\delta$'s are so similar: Essentially one has to replace $L$ by $\frac{1}{2}+(\vec{L}^2+\frac{1}{2})^{1/2}$ to obtain the quantum phase shift. In the Coulomb case we have chosen $\Phi^0$ such that there is no additional term depending only on $p$. Such a contribution only enters into the time delay and depends on the choice of $\Phi^0$. $\Phi$ determines $\delta$ up to a function of $p$ only. Also quantum mechanically the Coulomb phase shift can be deduced up to a function of $p$ by studying the asymptotic properties of $\Phi$.[11]

(3) The change in $\Phi^0$ does not repair Levinson's theorem for the Coulomb potential. Also the analog of Hellmann-Feynman's theorem and therefore the sign rule are not valid in this case. Note that now for $e^2>0$ (repulsive case) we have $\tau<0$ whereas for $V=e^2r^{-\nu}$, $\nu>1$, we get according to Eq. (6) of Sec. II that

$$\tau=\frac{e^2}{E}(2-\nu)\int_{-\infty}^{\infty}dt\,r(t)^{-\nu}.$$

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