Nonuniqueness of the Phase Shift in Central Scattering due to Monodromy

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Scattering at a central potential is completely characterized by the phase shifts which are the differences in phase between outgoing scattered and unscattered partial waves. In this Letter, it is shown that, for 2D scattering at a repulsive central potential, the phase shift cannot be uniquely defined due to a topological obstruction which is similar to *monodromy* in bound systems.

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Introduction.—In physics, it is often crucial to find ''suitable'' coordinates. One important set of coordinates in Hamiltonian mechanics is given by action-angle variables [1]. Action-angle variables played a crucial role in the development of early quantum mechanics in the Bohr-Sommerfeld quantization rule. The existence of action-angle variables was already addressed by Einstein in 1917 [2]. He argued that a quantization of actions only works if the mechanical system is integrable; i.e., it has as many independent constants of motion in involution as degrees of freedom. The existence of action-variables was made more precise in the Liouville-Arnold theorem [3]: if a connected component of the common level set of the constants of motion is regular (i.e., the gradients of the constants of motions are everywhere linearly independent on the component) and bounded, then it has the topology of a torus and action-angle variables exist in the neighborhood of the torus. The angles are the coordinates on the individual tori (which are just Cartesian products of circles), and the actions change from torus to torus in a smooth way. This theorem is local near a regular torus. If and how these ''local action-angle variables'' fit together *globally* has been ignored for a long time. Recently, it has been shown that there can exist topological obstructions to the global uniqueness of action-angle variables [4]. Consider a family of regular invariant tori in phase space that starts and ends with the same torus. This family may be a nontrivial torus bundle. Similarly, a Möbius strip is a nontrivial interval bundle: even though every local piece of it is just a rectangle, globally it is twisted. If the action variables are changed by a nontrivial unimodular transformation after one (mono) circuit (dromos) through a family of regular invariant tori, then the system has *monodromy*. Monodromy implies that the action-angle variables do *not* give global coordinates. It is a topological obstruction because the twist in the bundle cannot be removed by smooth deformations of the bundle. By contrast, if the loop of regular tori can be contracted (passing only through regular tori) it cannot have monodromy. In this way, monodromy is related to a nonregular level set of the constants of motion that is not a torus. Such critical sets appear in phase space where the gradients of the constants of motion are linearly dependent. The most prominent example of a critical set that causes monodromy is a pinched torus [5]. It exists in integrable systems with 2 degrees of freedom that have an unstable equilibrium point of focus-focus type, i.e., with eigenvalues of the form $\alpha \pm i\omega$, $-\alpha \pm i\omega$. One of the simplest examples with this type of monodromy is the spherical pendulum [5]. The quantum version of this phenomenon [6] explains why there is no global quantum number assignment for the hydrogen atom in external fields [7], the H_2^+ molecular ion [8], the rovibrational spectrum of CO_2 [9], and other systems [10].

In this Letter, we study the implication of the unbounded analog of monodromy in scattering problems. Elastic scattering at a central potential is completely characterized by the phase shifts which are the differences in phase of outgoing *scattered* partial waves and outgoing *unscattered* partial waves. For a planar system, a partial wave $\langle x, y|l, p\rangle$ with angular momentum l and asymptotic momentum p at infinity gains a phase $\delta(l, p)$. In fact, the action of the scattering matrix S on a partial wave is

$$S|l, p\rangle = \exp[2i\delta(l, p)]|l, p\rangle. \quad (1)$$

All physical quantities such as scattering cross sections and amplitudes can be expressed in terms of $\delta(l, p)$.

The phase shift is positive for attractive potentials and negative for repulsive potentials. If there is no interaction, then $\delta(l, p) = 0$. Similarly, the phase shift vanishes in the limiting case of large p where the potential can be ignored due to the dominating kinetic energy. The common procedure to define the phase shift therefore is to smoothly continue $\delta(l, p)$ from large to small p. We will show that for smooth repulsive potentials, there is a topological obstruction to this procedure, and as a consequence, the phase shift cannot be uniquely defined.

Nonuniqueness of phase shift.—Consider a smooth repulsive central potential $V(r)$ with $V(r) \to 0$ sufficiently fast for $r \to \infty$. The Taylor expansion at the origin is $V(r) = E_c - \mu\alpha^2 r^2/2 + \mathcal{O}(r^4)$ with $E_c > 0$. A semiclassical expression for $\delta(l, p)$ can be obtained from the WKB method [11]. Assuming $\delta(l, p) \to 0$ for $p \to \infty$, the WKB approximation yields $\delta_{\mathrm{WKB}}(l, p) = \Delta W(l, p)/(2\hbar)$ where $\Delta W(l, p)$ is the difference of the radial actions with and without potential,

$$\begin{aligned}\Delta W(l, p) &= W(l, p) - W'(l, p) \\ &:= 2\int_{r_0}^{\infty} \sqrt{p^2 - l^2/r^2 - 2\mu V(r)}\, dr \\ &\quad - 2\int_{r_0'}^{\infty} \sqrt{p^2 - l^2/r^2}\, dr. \end{aligned} \tag{2}$$

Here, r_0 and r_0' are the classical turning points with and without potential; i.e., r_0 is the largest nonnegative root of $r^2p^2 - l^2 - 2\mu r^2 V(r)$ or zero if $l = 0$ in combination with $p > p_c = (2\mu E_c)^{1/2}$, and $r_0' = |l|/p$. The difference ΔW is finite while the individual integrals diverge (see Fig. 1).

Surprisingly, the function $\Delta W(l, p)$ is not globally smooth: it is not differentiable at $l = 0$ when $p < p_c$. To illustrate this, we show contours of ΔW in Fig. 2(a). Consider the derivative of ΔW with respect to l,

$$\begin{aligned}\frac{\partial}{\partial l}\Delta W(l, p) &= \frac{\partial W(l, p)}{\partial l} - \frac{\partial W'(l, p)}{\partial l} \\ &= l\int_{z_0}^{\infty} \frac{-1}{z\sqrt{zp^2 - l^2 - 2\mu z U(z)}}\, dz \\ &\quad - l\int_{z_0'}^{\infty} \frac{-1}{z\sqrt{zp^2 - l^2}}\, dz. \end{aligned} \tag{3}$$

Here, we substituted $z = r^2$ and let $U(z) \equiv V(\sqrt{z})$. In contrast to the integrals in (2), their derivatives with respect to l exist individually. The second integral is elementary and gives $-\mathrm{sgn}(l)\pi$.

For general l and p, the integral $\partial W(l, p)/\partial l$ in (3) depends on the potential U. Interestingly, for $l = 0$, this is no longer the case. The limiting case $l \to 0$ is tricky: depending on whether $p > p_c$ or $p < p_c$ the branch point z_0 of the square root in the integrand either collides or does not collide with the integrand's pole at $z = 0$ as $l \to 0$. The collision of the branch point and the pole leads to the divergence of the integral, and the question arises of how this divergence is compensated by the vanishing of the prefactor l. At $z = 0$, the argument of the square root has the Taylor expansion

$$-l^2 + (p^2 - p_c^2)z + \mu^2\alpha^2 z^2 + \mathcal{O}(z^3). \tag{4}$$

We note that in case $\alpha = 0$, higher order terms can be included and do not lead to a substantial change of the following argument. For $p < p_c$, the linear term of this expression has a negative coefficient that does not depend on l. Hence, the collision of z_0 and zero as $l \to 0$ does not take place, and the integral is not critical in this limiting case. Because of the prefactor l in (3), we thus have $\partial W(l, p)/\partial l \to 0$ as $l \to 0$ and accordingly, the left and right hand derivatives of $\Delta W(l, p)$ with respect to l at zero are

$$\lim_{l \to 0^{\mp}} \frac{\partial \Delta W(l, p)}{\partial l} = \mp\pi \quad (p < p_c). \tag{5}$$

When $p > p_c$, the coefficient of the linear term in (4) is positive, and the collision of the branch point and the pole *does* take place. Consider the integral in the complex plane. For $l \neq 0$, we define the integration path C as shown in

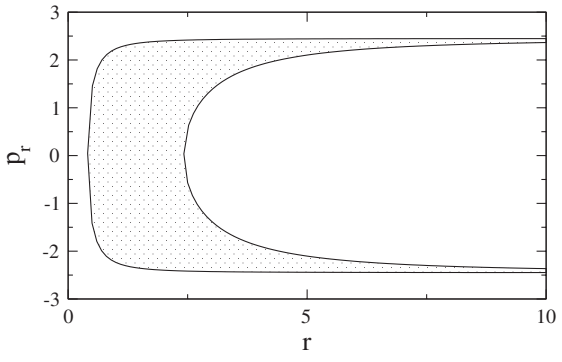

FIG. 1. Phase portrait $(r,\ p_r)$ with $p_r^2 = 2\mu E - l^2/r^2 - 2\mu V(r)$ with $E = 3$, $l = 1$, and $V(r) \equiv 0$ (outer curve) and $V(r) = a/[1 + (br)^2]$ with $a = 20$ and $b = 1$ (inner curve). The shaded area is equal to ΔW defined in (2).

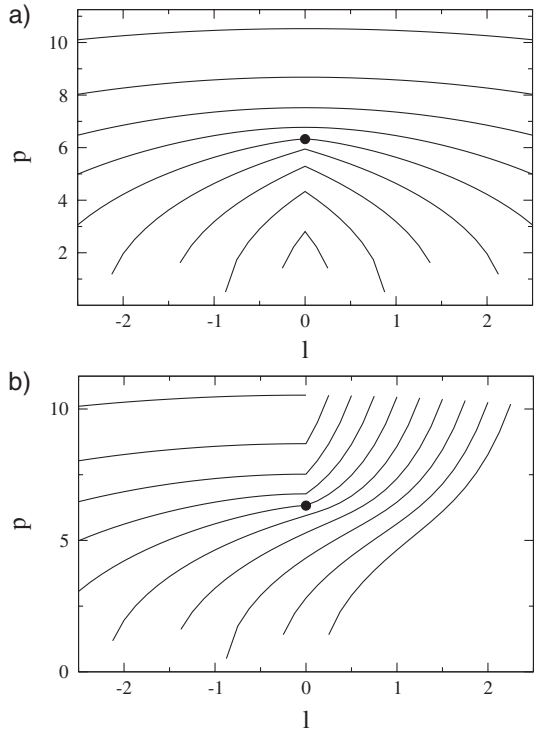

FIG. 2. (l, p)-plane with contours of (a) ΔW defined in (2) and (b) $\Delta\tilde{W}$ defined in (10). The bold dot marks $(l, p) = (0, p_c)$. The potential is the same as in Fig. 1.

Fig. 3. This gives

$$\frac{\partial W(l,p)}{\partial l} = l\int_C \frac{-1}{2z\sqrt{zp^2 - l^2 - 2\mu z U(z)}}dz. \quad (6)$$

To study the limit $l \to 0$, we deform the integration path C by wrapping it over the pole at zero and compensate the capture of the pole by adding a small closed integration path that encircles the pole in opposite direction. Thus, we decompose $C = C_1 + C_2$ with C_1 and C_2 as shown in Fig. 3. The integral (6) thus becomes

$$\frac{\partial W(l,p)}{\partial l} = \sum_{k=1}^{2} l\int_{C_k} \frac{-1}{2z\sqrt{zp^2 - l^2 - 2\mu z U(z)}}dz. \quad (7)$$

The integration path C_1 is not critical for $l \to 0$, and due to the prefactor l, the contribution to $\partial W/\partial l$ vanishes for $l \to 0$. For the choice of the branch of the square root explained in Fig. 3, the differential $-dz/[2z\sqrt{zp^2 - l^2 - 2\mu z U(z)}]$ has residue $-i/(2|l|)$ at $z = 0$. The integral along C_2 thus leads to the contribution

$$l\int_{C_2} \frac{-1}{2z\sqrt{zp^2 - l^2 - 2\mu z U(z)}}dz = \mathrm{sgn}(l)\pi. \quad (8)$$

We thus find that for $p > p_c$, the contributions of $\partial W(l,p)/\partial l$ and $\partial W'(l,p)/\partial l$ to $\partial \Delta W(l,p)/\partial l$ cancel each other for $l \to 0$ and, accordingly,

$$\lim_{l\to 0} \frac{\partial}{\partial l}\Delta W(l,p) = 0 \quad (p > p_c). \quad (9)$$

One might think of removing the kink in Fig. 2(a) by "smoothing" $\Delta W(l,p)$ according to

$$\Delta\tilde{W}(l,p) = \begin{cases} \Delta W(l,p) & \text{for } l \le 0 \\ \Delta W(l,p) - 2\pi l & \text{for } l > 0 \end{cases}. \quad (10)$$

This however introduces a kink at the segment of $l = 0$ where $p > p_c$, see Fig. 2(b).

The WKB method gives $2\hbar\delta = \Delta W$ where $l = m\hbar$, $m \in \mathbb{Z}$. The values of δ are only relevant mod π, see (1). In other words, the function $\exp(2i\delta)$ is (locally) periodic. In order to study this periodicity, we consider the values $p = k\hbar$ such that $\delta(m\hbar, k\hbar) = 0 \bmod \pi$, see Fig. 4. The function $\exp(2i\delta)$ is not globally periodic because of the singularity at $(m,k) = (0, p_c/\hbar)$. This can be seen by transporting a unit cell in the lattice around the singularity. The lattice cell crosses the line $m = 0$ according to the modified $\Delta\tilde{W}$ of (10) which is smooth for $p < p_c$, while the original ΔW is smooth for $p > p_c$. Thus, in the presence of a repulsive localized potential, the phase shift δ cannot be globally defined. We call this phenomenon *quantum scattering monodromy*.

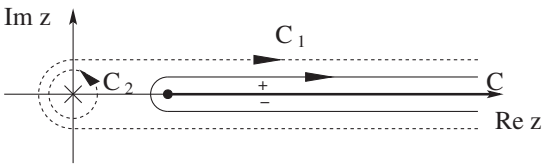

FIG. 3. Complex z-plane with integration paths for the differential $-dz/\{2z[zp^2 - l^2 - 2\mu z U(z)]^{1/2}\}$ which has a pole at the origin $z = 0$ (marked by the cross). The square root is real along the branch cut which extends from the turning point z_0 (marked by the dot) along the positive real axis; it is positive "above" and negative "below" this branch cut. The integration path C (solid line) is equivalent to the composition $C = C_1 + C_2$ (dashed line).

Notice that the derivative of the phase shift with respect to the energy gives the eigenvalues of the Wigner-Smith time delay matrix $Q = -i\hbar S^{-1}\partial S/\partial E$. Semiclassically, this derivative is given by $\partial\Delta W(l,p)/\partial E = \Delta T$ which is the classical time delay. This derivative is smooth everywhere apart from the point $(l,E) = (0, E_c)$.

The WKB approximation (2) does not account for the collision of the classical turning point and the singularity of the effective potential when $l \to 0$. An asymptotic expansion of the exact solution of the radial wave equation shows that nevertheless the error is less than 1%.

Classical explanation.—The classical interpretation of $\partial\Delta W(l,p)/\partial l$ is the angle of deflection. Consider the polar angle φ between the incoming and outgoing orbit in configuration space,

$$\varphi = \int_{-\infty}^{\infty} \dot{\varphi} dt = \int_{-\infty}^{\infty} \frac{l}{\mu r^2} dt. \quad (11)$$

Substituting $dt = dr/\dot{r}$ gives

$$\varphi = \int_{\infty}^{r_0} \frac{l}{\mu r^2}\frac{1}{\dot{r}}dr + \int_{r_0}^{\infty} \frac{l}{\mu r^2}\frac{1}{\dot{r}}dr \quad (12)$$

$$= 2\int_{r_0}^{\infty} \frac{l}{r\sqrt{2\mu E r^2 - l^2 - 2\mu r^2 V(r)}}dr \quad (13)$$

where r_0 is the turning point. We used $\dot{r} < 0$ in the first integral and $\dot{r} > 0$ in the second integral in (12). Up to the sign, the derivative $\partial\Delta W(l,p)/\partial l$ in (3) thus coincides

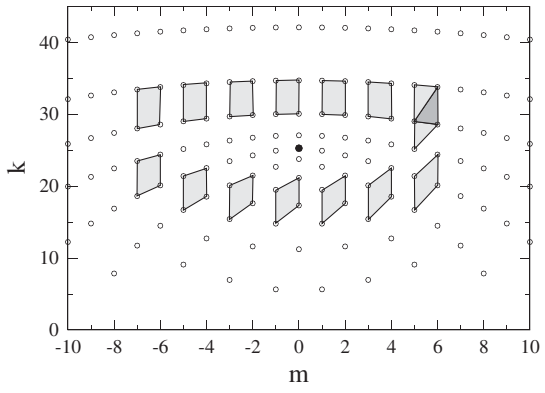

FIG. 4. Lattice of zeros (empty circles) of the phase shift δ mod π in the plane $m = l/\hbar$, $k = p/\hbar$, and parallel transport of a lattice cell about the singularity $(m,k) = (0, p_c/\hbar)$ (filled circle). The potential is the same as in Fig. 1. $\hbar = 0.25$.

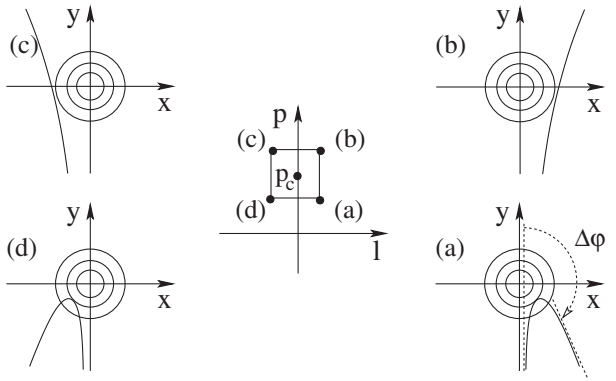

FIG. 5. Orbits in configuration space coming in from $y = -\infty$ for four different pairs of angular momenta and asymptotic momenta marked as bold points on the path in the (l, p)-plane that encircles the critical point $(l, p) = (0, p_c)$.

with the angle of deflection $\Delta\varphi$ between the scattered and the corresponding unscattered orbit.

Let us now follow the deflection angle $\Delta\varphi$ for pairs of angular momenta (or equivalently impact parameters) and asymptotic momenta (i.e., energies) along a closed path in the (l, p)-plane that encircles the critical point $(l, p) = (0, p_c)$, see Fig. 5. Consider orbits that come in from $y = -\infty$. For $l = 0$ and $p < p_c$, the particle comes in along the y-axis and slows down. Because of insufficient energy, it cannot overcome the potential barrier and so turns back towards $y = -\infty$. This orbit has $\Delta\varphi = \pi$. If l is increased to a value $l = l_{(a)} > 0$ (keeping $p < p_c$ fixed), then the particle gets deflected to the right, and $\Delta\varphi$ decreases to a value $\pi > \Delta\varphi_{(a)} > 0$. If we now increase p to a value $p_{(b)} > p_c$ (keeping l fixed), the deflection angle $\Delta\varphi$ decreases to a value $0 < \Delta\varphi_{(b)} < \Delta\varphi_{(a)}$. If we then decrease l (keeping p fixed), the deflection angle decreases further. At $l = 0$, the particle comes in along the y-axis, slows down, but now has sufficient energy to cross the barrier and move towards $y = +\infty$. This orbit has $\Delta\varphi = 0$. If l is decreased further to a negative value $l_{(c)} < 0$, the particle gets deflected to the left giving a negative deflection angle $-\pi < \Delta\varphi_{(c)} < 0$. If p is then decreased to a value $p_{(d)} < p_c$ (keeping l at $l_{(c)} < 0$), the defection angle decreases further to a value $-\pi < \Delta\varphi_{(d)} < \Delta\varphi_{(c)}$. If l is increased (keeping p fixed at $p_{(d)}$), the deflection angle decreases even further, and at $l = 0$, it reaches the value $\Delta\varphi = -\pi$. Upon returning to the starting point of the closed path γ in the (l, p)-plane that encircles the critical point $(l, p) = (0, p_c)$, the deflection angle thus is increased by 2π,

$$\oint_\gamma \frac{\partial \Delta W(l, p)}{\partial l} dl + \frac{\partial \Delta W(l, p)}{\partial p} dp = 2\pi. \qquad (14)$$

Such a nonzero value from a closed loop γ only occurs when the critical point $(0, p_c)$ is encircled by γ. If a system has loops of regular values for which the deflection angle is increased by (multiples of) 2π, we say the system has *scattering monodromy.*

For the classical system, the angular momentum L and the Hamiltonian function H are two independent constants of motion which are in involution. The classical system is therefore integrable. The level set $\{L = l, H = E\}$ in phase space for a regular value (l, E) topologically is a cylinder. The invariant cylinder $\mathbb{R} \times S^1$ consists of an orbit ($\sim\mathbb{R}$) as shown in Fig. 5 and all its partners with different angle of incidence ($\sim S^1$) but the same l and E. At the critical value $(0, E_c)$, the gradients of L and H are linearly dependent. The critical level set $\{L = 0, H = E_c\}$ is topologically a cone. It consists of the equilibrium point at the origin and all orbits approaching it forward or backward in time. The invariant cone (a pinched cylinder) in the phase space of a scattering system is the analogue of the pinched torus in a bound system. A loop of invariant cylinders that encircles the invariant cone cannot be contracted, and as a result, $\Delta\varphi$ shows scattering monodromy.

Conclusions.—We have shown that the quantum scattering phase shift δ for a smooth radially symmetric repulsive potential cannot be globally defined. The classical analogue is that the deflection angle changes by 2π upon traversing a loop in the space of constants of motion that encloses the critical value corresponding to the equilibrium point. As opposed to the more abstract consequences of monodromy in compact systems, this phenomenon is ''directly'' observable, e.g., by playing marbles (neglecting moments of inertia) on a surface with a rotationally symmetric bump.

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