REFLECTION OF A SELF-PROPPELLING RIGID DISK
FROM A BOUNDARY

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Abstract. A system of ordinary differential equations that describes the motion of a self-propelling rigid disk is studied. In this system, the disk moves along a straight-line and reflects from a boundary. Interestingly, numerical simulation shows that the angle of reflection is greater than that of incidence. The purpose of this study is to present a mathematical proof for this attractive phenomenon. Moreover, the reflection law is numerically investigated. Finally, existence and asymptotic stability of a square-shaped closed orbit for billiards in square table with inelastic reflection law are discussed.

1. Introduction. Self-propelling motions have been attracting more and more research interests in various areas of sciences [13, 21]. A camphor scrapping floating on water is a concrete example of a self-propelling rigid body, which obtains the driving force by making the surface tension around the camphor scrapping inhomogeneous [27], [23], [19]. In these decades, camphor motions have been studied from both mathematical and experimental viewpoints [20], e.g., the occurrence of camphor motion ([17], [1]), motions of asymmetry shape ([19], [18], [7], [3]), and collective motions of many camphor boats [2], [8]. However, motions of a camphor disk are not fully understood from the viewpoint of mathematics.

If the camphor scrapping is disk-shaped, then one can observe billiard-like motion on a relatively large water vessel [1], that is, the disk corresponding to a billiard ball repeats motion in a straight line and reflection from the boundary. There are, however, some essential differences from billiards as a sport: (i) The disk reflects without collision with the boundary, and (ii) the angle of reflection is greater than
that of incidence. See Fig. 1(A). These properties appear in the reflection of a self-propelling particle [22, 25]. As a consequence of these properties, motions in square or rectangular domains are quite different from the one in mathematical billiards [14, 15].

![Figure 1](image_url)

**Figure 1.** (A) A laboratory experiment of camphor motions. (B) A trajectory of the center of the disk governed by the moving boundary model (7) below.

For example, numerical simulations suggest that a typical trajectory in square approaches to a square-shaped periodic orbit such that the disk visits each edge of the square in turn (Fig. 1(B)), while the trajectory in mathematical billiards is periodic or dense in the square sensitively depending on the initial data [24, Chapter 2]. It is natural to consider that the property (ii) above is responsible for this difference in motions. We will see below, however, that it is not sufficient for the stability of a square-shaped periodic orbit. What is the relation between the reflection rule and the trajectory? Before coping with this question, we have to make clear what kind of reflection rules can be realized in motion of a self-propelling rigid disk. The property (ii) above will be one of the most fundamental assumptions on the reflection rules. In spite of its importance, it has not been proved with mathematical rigor. In this paper, we study the reflection of a camphor disk to prove the property (ii).

We consider a particle model in the half-plane \( \{ (x, y) \in \mathbb{R} \mid x > 0 \} \) [4, 1], which was derived as the motion of the center of the camphor disk:

\[
\begin{align*}
\dot{x} &= v + m_0 h(x), \\
\dot{y} &= w, \\
\dot{v} &= \left[ \delta - (v^2 + w^2) \right] v + m_2 h(x), \\
\dot{w} &= \left[ \delta - (v^2 + w^2) \right] w,
\end{align*}
\]

where \((x(t), y(t))\) denotes the center position of the camphor disk, \((v(t), w(t))\) are related to the velocity, the dots mean differentiation with respect to a time variable \(t\), \(\delta > 0\), \(m_0 \geq 0\), \(m_2 > 0\) are parameters. Note that a solution of (1) with \(\delta > 0\) and \(m_0 = m_2 = 0\), which corresponds to a free motion on the entire plane, converges to motion in a straight-line with a constant speed \(\sqrt{\delta}\) as \(t \to \infty\). \(h(x)\) is positive-valued, monotonically decreasing, and \(C^2\)-class on \((0, \infty)\), and a typical case is...
We will give assumptions on $h$ in Assumption 2 below. We briefly explain the derivation of this model in the next section. In this model equation (1), a very attractive phenomenon in which the angle of reflection against the boundary $\{x = 0\}$ is greater than that of incidence was numerically observed [11, 14, 15]. See Fig. 2(A).

The purpose of this paper is to derive the relation on angles theoretically from the model equation (1).

Introducing new variables $z, r, \text{ and } \theta$ by

$$z = h(x), \quad v = r \cos \theta, \quad w = r \sin \theta,$$

we obtain

$$\begin{cases}
\dot{z} = H(z)(r \cos \theta + m_0 z), \\
\dot{r} = (\delta - r^2) r + m_2 z \cos \theta, \\
\dot{\theta} = -\frac{m_2 z}{r} \sin \theta,
\end{cases}$$

where $H(z)$ is an extension of $h'(h^{-1}(z))$ as an odd function on $\mathbb{R}$ and is defined by

$$H(z) = \begin{cases} 
\text{sgn}(z)h'(h^{-1}(\text{sgn}(z)z)) & (z \neq 0), \\
0 & (z = 0).
\end{cases}$$

This makes sense because $h(x)$ is monotone in $x \in (0, \infty)$. Since $(\dot{x}, \dot{v}, \dot{w})$ is independent of $y$, we only have to study (4).

We consider entire solutions of (4) satisfying the following condition for some $\theta_{-\infty}$ and $\theta_{\infty}$:

$$\lim_{t \to \pm \infty} (z(t), r(t), \theta(t)) = (0, \sqrt{\delta}, \theta_{\pm \infty}).$$

Such a solution does exist as we shall show below. Let us define the angles of incidence and reflection as follows (see Fig. 2(B)).

**Definition 1.1.** Suppose that there exists a solution of (1) satisfying (5) for some $\theta_{-\infty}$ and $\theta_{\infty}$. Then the angle of incidence and that of reflection are defined by

$$\theta_{\text{inc}} = \pi - \theta_{-\infty}, \quad \theta_{\text{ref}} = \theta_{\infty},$$
respectively.

If \( \theta_{-\infty} \) lies on the interval \([\pi/2, \pi]\), then \( \theta_{\text{inc}} \) is the angle formed by vectors \((v, w) = \sqrt{3}(\cos \theta_{-\infty}, \sin \theta_{-\infty}) \) and \((-1, 0)\). On the other hand, if \( \theta_{\infty} \in [0, \pi/2] \), then \( \theta_{\text{ref}} \) is the angle formed by vectors \((v, w) = \sqrt{3}(\cos \theta_{\infty}, \sin \theta_{\infty}) \) and \((1, 0)\). Since \( \dot{x} \rightarrow v \) as \( x \rightarrow \infty \) and \( \dot{y} = w \), these definitions are appropriate for understanding reflection of a particle governed by (1).

In the present paper, we assume the following unless we say otherwise.

**Assumption 1.** \( \delta > 0 \) and \( m_0 = 0 \).

As mentioned above, \( \delta > 0 \) is necessary for the occurrence of motion. We assume \( m_0 = 0 \) just for a technical reason, which should be removed in a future study. The next is one of assumptions on \( h(x) \), which is a generalization of (2):

**Assumption 2.** The function \( h(x) \) is a \( C^2 \) function on \((0, \infty)\) which satisfies the following conditions:

(A1) \( h(x) > 0 \) for any \( x > 0 \),

(A2) there exists \( a > 0 \) such that \( h'(x) \leq -ah(x) \) for any \( x > 0 \),

(A3) \( h''(x) > 0 \) for any \( x > 0 \),

(A4) \( h'(x) \rightarrow 0 \) as \( x \rightarrow \infty \), and

(A5) there exists \( c > 0 \) such that \( h''(x)/h'(x) \rightarrow -c \) as \( x \rightarrow +\infty \).

Here is the main theorem of this study:

**Main Theorem.** Suppose that \( \theta_{-\infty} \) is in the interval \([\pi/2, \pi]\). The followings hold:

(I) There exist \( \theta_{\infty} \in [0, \pi/2] \) and a solution of (4) satisfying (5).

(II) \( \sin \theta_{-\infty} \leq \sin \theta_{\infty} \) holds, where the equality holds only if \( \theta_{-\infty} = \pi \) or \( \theta_{-\infty} = \pi/2 \).

(III) If \( \theta_{-\infty} \neq \pi/2 \), then \( v(t) \) changes its sign from negative to positive just once. Accordingly, \( \theta_{\text{ref}} \) is a function of \( \theta_{\text{inc}} \). Moreover, \( \theta_{\text{inc}} \leq \theta_{\text{ref}} \) holds, where the equality holds only if \( \theta_{\text{inc}} = 0, \pi/2 \).

\( \theta_{\text{inc}} = 0 \) is the case where the trajectory of the particle is along a normal line of the boundary \( \{x = 0\}\). \( \theta_{\text{inc}} = \pi/2 \) corresponds to the case where the particle moves at \( x = \infty \) along a parallel line to the boundary, that is, a reflection never occurs.

The rest of the present paper is organized as follows. In the next section, we explain the derivation of (1) from a PDE model. Section 3 is devoted to the proof of the Main Theorem. In Section 4, the relation \( \theta_{\text{ref}} = F(\theta_{\text{inc}}) \) is numerically investigated. Finally, we discuss a discrete-time model which describes billiard motions governed by a reflection law \( \theta_{\text{ref}} = F(\theta_{\text{inc}}) \) with \( \theta_{\text{ref}} > \theta_{\text{inc}} \).

2. **Mathematical models.** In this section, we briefly explain how to derive (1) from a PDE model [1]. We refer to [1] for derivation of the PDE model based on the knowledge of chemistry.

First, we introduce a mathematical model for motions of a single camphor disk [1]. The camphor disk at time \( t \) is represented by the disk centered at \( p(t) = (p_1(t), p_2(t)) \) with the radius \( r_0 \), i.e., \( B(t) = \{x = (x_1, x_2) \in \mathbb{R}^2 \mid |x - p(t)| \leq r_0\} \). Let \( \Omega \subseteq \mathbb{R}^2 \) be the water vessel. The equations of motion are:

\[
\begin{align*}
\partial_t u &= D \Delta u - ku + f(u)\chi_{B(t)}, \quad x \in \Omega, \ t > 0 \\
\dot{p} &= \beta \int_{\partial B(t)} \gamma(u(t, x))v ds, \quad t > 0,
\end{align*}
\] (7)
where \( u(t, x) \) is the concentration of camphor molecules dissolved into water, \( \Delta \) is the two-dimensional Laplacian, \( f \) is a non-increasing and nonnegative function for \( u \geq 0 \), \( \chi_{B(t)} \) is the characteristic function on \( B(t) \), \( \nu \) is the outward unit normal on \( \partial B(t) \), and \( D, k, \) and \( \beta \) are positive constants. \( \gamma(u) \) is a function given by

\[
\gamma(u) = \frac{\gamma_0}{1 + au}
\]

with positive constants \( \gamma_0 \) and \( a \), which represents the surface tension. The Neumann boundary condition is imposed on \( \partial \Omega \). This model describes that camphor molecules dissolve into water and diffuse, by which the surface tension decreases. The camphor disk is pulled to the region where the surface tension is relatively high. Figure 3 shows a trajectory of \( p(t) \) starting at \( p(0) = (-75, 0) \) on the domain \( \Omega = [-80, 80] \times [-20, 20] \). Clearly, the disk exhibits billiard-like motion and the angle of reflection gets greater and greater.

![Figure 3. A trajectory of the center of the disk governed by the moving boundary model (7). Parameters are \( r_0 = 1.0, D = 0.13, k = 1.0, \beta = 1.0, \gamma_0 = 1.0, a = 2.0, \) and \( F(u) \equiv 2.0 \).](image)

A particle model which describes free motions on \( \Omega = \mathbb{R}^2 \) is derived in the following way. Introducing new variables by \( y = x - p(t) \) and \( U(t, y) = u(t, y + p(t)) \), we transform (7) to a single nonlocal equation:

\[
\partial_t U = D \Delta U - kU + \beta \int_{|y| = r_0} \gamma(U) \nu ds \cdot \nabla U + f(U) H(r_0 - |y|),
\]

where \( H \) is the Heaviside function and \( \nu \) is the unit outward normal vector of the circle \( \{|y| = r_0\} \). Note that this equation is independent of \( p \) and that \( p \) is obtained by integrating

\[
\dot{p} = \beta \int_{|y| = r_0} \gamma(U) \nu ds.
\]

Let \( S : [0, \infty) \to \mathbb{R}, r \mapsto S(r) \) be a solution of

\[
\begin{cases}
D(S'' + r^{-1} S') - kS + f(S) H(r_0 - r) = 0, & r \in [0, \infty) \\
S'(0) = 0, & S(\infty) = 0.
\end{cases}
\]

Then \( (u(t, x), p(t)) = (S(|x|), 0) \) is a stationary solution of (7), which corresponds to the rest state of a camphor disk. The linear stability of this rest state is determined by the spectrum of linearized operator of (8) about \( U(t, x) = S(|x|) \). Suppose that \( S \) satisfies \( S(r) \to r^{-1/2} \exp(-kr)b \) as \( r \to +\infty \) for some nonzero constant \( b \). Chen et al. [1] proved that there exists \( \beta = \beta^* \) at which a drift bifurcation occurs to
bifurcate a traveling spot solution for $\beta > \beta_*$. The bifurcation equation for this bifurcation is given by
\[
\dot{p} = \zeta, \quad \dot{\zeta} = (\delta - M_1|\zeta|^2) \zeta, \quad (10)
\]
where $\delta \propto \beta - \beta_*$ is a bifurcation parameter, and $M_1$ is a constant determined by the parameters in (7). Thus the motion of a camphor disk is completely described by equations for its center position and velocity, provided that the parameter is sufficiently close to the bifurcation point.

Next, we consider interactions of two camphor disks of the same radius $r_0$, whose centers at time $t$ are $p_1(t)$ and $p_2(t)$, respectively. Let $B_j(t) = \{x \mid |x - p_j(t)| \leq r_0\}$ for $j = 1, 2$. The equations of motion are given by
\[
\begin{cases}
\partial_t u = D \Delta u - ku + f(u) \chi_{B_1(t)} + f(u) \chi_{B_2(t)}, \quad x \in \mathbb{R}^2, t > 0 \\
\dot{p}_j = \beta \int_{\partial B_j(t)} \gamma(u(t, x)) \nu ds \quad (j = 1, 2), \quad t > 0.
\end{cases}
\]
(11)

Let $d = p_2 - p_1$. If $\beta$ is sufficiently close to the bifurcation point $\beta_*$, then $p_1$ and $p_2$ are governed by
\[
\begin{cases}
\dot{p}_j = \zeta_j - M_0 e^{-k|d|} \frac{(p_{j+1} - p_j)}{|d|}, \\
\dot{\zeta}_j = (\delta - M_1^*|\zeta_j|^2) \zeta_j - M_2^* e^{-k|d|} \frac{(p_{j+1} - p_j)}{|d|},
\end{cases}
\]
(12)
for $j = 1, 2$, where $p_{2+1}$ is identified with $p_1$, and $M_0^*, M_1^*$, and $M_2^*$ are constants determined by the parameters in (7).

Finally we explain the derivation of (1). Let $p_2(t) = (x(t), y(t))$ and $\zeta_2(t) = (v(t), w(t))$. It is easy to see that $p_1(0) = (-x(0), y(0))$ and $\zeta_1(0) = (-v(0), w(0))$ imply $p_1(t) = (-x(t), y(t))$ and $\zeta_1(t) = (-v(t), w(t))$ for all $t > 0$. Therefore the particle $(p_1, \zeta_1)$ is the mirror image of $(p_2, \zeta_2)$ throughout. We regard the interaction between these two particles as the repulsive interaction of $(p_2, \zeta_2)$ and the boundary $\{x, y \mid x = 0\}$. Moreover, we only have to solve equations for $(x, y, v, w)$ to study the reflection from the boundary. We obtain (1) by rescaling variables and replacing the interaction terms by more general form. For the moving boundary model on the half-plane $\{x_1 \geq 0\}$ with the Neumann boundary condition, it is possible to obtain (12) with remainder terms with a mathematical rigor. In fact, model equations with the Neumann boundary condition on the half-plane $\{x_1 \geq 0\}$ can be equivalently reduced to the problems on the whole plane without boundary conditions by restricting to symmetric functions with respect to $x_1 = 0$. In this sense, considering the mirror image is a rigorous identification. It should be noted, however, that this study focuses on the truncated system (12), that is, an approximate system.

3. Proof of main theorem. Throughout this section, we assume that Assumptions 1 and 2 hold. We use the following properties of $H(z)$:

**Lemma 3.1.** $H(z)$ is a monotone decreasing $C^1$ function on $\mathbb{R}^2$, $H(z) \leq -az$ holds for $z \geq 0$, and $H'(0) = -c < 0$, where $a$ and $c$ are the constants appearing in Assumption 2.

**Proof.** From the second and fourth conditions of Assumption 2, we obtain $H(z) \leq -az$ for $z \geq 0$. It is easy to see that $H'(z) = h''(h^{-1}(z))/h'(h^{-1}(z))$ for $z > 0$. By assumption, it turns out that $H'(z)$ converges to $-c$ as $z$ tends to zero from right.
Since $H'(z)$ is even, we obtain $H'(z) \to -c$ as $z \to 0$. Thus $H$ is $C^1$ on $\mathbb{R}$. As $h'(x) < 0$ and $h''(x) > 0$ for any $x > 0$, $H'(z) < 0$ for any $z \in \mathbb{R}$.

Let us begin with easy cases.

**Lemma 3.2.** Let $\theta_\infty = \pi/2$. Then $(z(t), r(t), \theta(t)) = (0, \sqrt{\delta}, \pi/2)$ is a solution of (4) satisfying (5) with $\theta_\infty = \pi/2$, and $\sin \theta_\infty = \sin \theta_\infty = 1$ holds.

**Proof.** $(z, r, \theta) = (0, \sqrt{\delta}, \pi/2)$ is an equilibrium of (4).

**Lemma 3.3.** Let $\theta_\infty = \pi$. Then there exists a heteroclinic solution of (1) from $(z, v, w) = (0, -\sqrt{\delta}, 0)$ to $(0, \sqrt{\delta}, 0)$. In this case $\theta_\infty = 0$ and $\sin \theta_\infty = \sin \theta_\infty = 0$.

**Proof.** If $\theta_\infty = \pi$, then $w = 0$. As the $(z, v)$-plane is invariant, we only have to consider the vector field on it, which is given by

$$
\dot{z} = H(z)v, \quad \dot{v} = (\delta - v^2) v + m_2 z. \tag{13}
$$

There are three equilibria $(z, v) = (0, 0)$ and $(0, \pm \sqrt{\delta})$. It is easy to see that $(0, -\sqrt{\delta})$ and $(0, \sqrt{\delta})$ are saddle points and stable nodes, respectively. The linearized eigenvalues of the origin are positive and zero.

We construct a closed positively invariant set for which we apply the Poincaré-Bendixson theorem. Notice that the $v$-axis is invariant. This implies that $\{(z, v) \mid z > 0\}$ is also invariant. Moreover, it turns out that the set $S = S_0 \cup S_1$ is positively invariant, where $S_0$ and $S_1$ are defined by

$$
S_0 = \{(z, v) \mid z \geq 0, v \geq 0\},
$$

$$
S_1 = \{(z, v) \mid m_2 z \geq v(v^2 - \delta), -\sqrt{\delta} \leq v \leq 0\}.
$$

To show this, let us observe the vector field on the boundary of $S$. If $z > 0$ and $v = -\sqrt{\delta}$, then $\dot{z}$ and $\dot{v}$ are positive. If $z > 0$, $v \in (-\sqrt{\delta}, 0)$ and $m_2 z = v(v^2 - \delta)$, then $\dot{z} > 0$ and $\dot{v} = 0$. Thus, $S$ is positively invariant. In addition, $S_0$ is also positively invariant because $\dot{z} = 0$ and $\dot{v} > 0$ if $z > 0$ and $v = 0$. Note that there exists $z_0 > 0$ such that the $\omega$-limit set of $(z_0, -\sqrt{\delta})$ is the equilibrium $(0, \sqrt{\delta})$. As long as $(z, v) \in S_1$, we have the inequality $\dot{v} \geq \delta v + m_2 z$. If $z_0 > \delta^{1/2}/m_2$, then the solution of

$$
\dot{v} = \delta v + m_2 z_0, \quad v(0) = -\sqrt{\delta}
$$

exponentially grows as time passes. Therefore, the solution of (13) with the initial value $(z(0), v(0)) = (z_0, -\sqrt{\delta})$ arrives at $z$-axis in a finite time. As $\dot{v} > 0$ for $z > 0$, $v = 0$, there exists $\varepsilon > 0$ and $t_1 > 0$ such that $v(t_1) = \varepsilon$. Since $H(z) \leq -az$ holds, we obtain $\dot{z} = H(z)v \leq -az$, and hence, $0 \leq z(t) \leq z(t_1)e^{-az(t-t_1)}$ for $t > t_1$. Therefore, $z(t)$ exponentially decays to zero. Since we have

$$
v(\delta - v^2) \leq \dot{v} \leq v(\delta - v^2) + m_2 z,
$$

$v(t)$ tends to $\sqrt{\delta}$ as $t \to \infty$. Thus, the $\omega$-limit set of $(z_0, -\sqrt{\delta})$ is $(0, \sqrt{\delta})$.

Let $D$ be the closed region bounded by the following four curves:

$$
\{(z, v) \mid 0 \leq z \leq z_0, v = -\sqrt{\delta}\},
$$

$$
\{(z, v) \mid m_2 z = v(v^2 - \delta), -\sqrt{\delta} \leq v \leq 0\},
$$

$$
\{(z, v) \mid z = 0, 0 \leq v \leq \sqrt{\delta}\},
$$

and the closure of the positive orbit of $(z_0, -\sqrt{\delta})$. Then $D$ is positively invariant. It turns out by phase-plane analysis that no cycle is contained in $D$. Therefore, the
Lemma 3.5. The subset that the $\omega$-limit set is an equilibrium for any initial point in $D$. Notice that the origin cannot attract any positive orbit from the interior of $D$: this is obvious from the phase-plane analysis and can be verified by the center manifold reduction. Hence, only $(0, \sqrt{\delta})$ is attractive in $D$.

One can take an initial value $(z_*, v_*)$ on the unstable manifold of the equilibrium $(z, v) = (0, -\sqrt{\delta})$ so that $(z_*, v_*)$ lies in the interior of $D$. Indeed, the eigenvector of the linearized matrix of (13) at $(0, -\sqrt{\delta})$ associated with the eigenvalue $\sqrt{\delta}$, which is tangent to the unstable manifold, is given by $(c\sqrt{\delta} + 2\delta, m_2)$, and $(c\sqrt{\delta} + 2\delta)/m_2 > 2\delta/m_2$ holds. Therefore, the orbit of $(z_*, v_*)$ is heteroclinic from $(0, -\sqrt{\delta})$ to $(0, \sqrt{\delta})$.

Next, we consider the case where $\theta_{-\infty} \in (\pi/2, \pi)$. The next lemma is straightforward.

Lemma 3.4. For any $\phi \in [0, 2\pi]$, $(z, r, \theta) = (0, \sqrt{\delta}, \phi)$ is an equilibrium of (4), whose eigenvalues are

$$0, \quad -2\delta, \quad -c\sqrt{\delta} \cos \phi.$$ 

The eigenspace associated with the eigenvalue $-c\sqrt{\delta} \cos \phi$ is

$$E^u(\phi) = \text{span} \left\{ 1, \frac{m_2 \cos \phi}{2\delta - c\sqrt{\delta} \cos \phi}, \frac{m_2 \tan \phi}{c\delta} \right\}.$$

Note that $-c\sqrt{\delta} \cos \theta_{-\infty}$ is positive for $\theta_{-\infty} \in (\pi/2, \pi)$. Hence, if we take an initial data $(z_0, r_0, \theta_0)$ on the unstable manifold of $(z, r, \theta) = (0, \sqrt{\delta}, \theta_{-\infty})$, then $(z(t), r(t), \theta(t))$ converges to $(0, \sqrt{\delta}, \theta_{-\infty})$ as $t$ tends to $-\infty$. It remains to show that the $\omega$-limit set of $(z_0, r_0, \theta_0)$ is $(0, \sqrt{\delta}, \theta_{-\infty})$ for some $\theta_{-\infty} \in (0, \pi/2)$.

Lemma 3.5. The subset $S = \{(z, r, \theta) \mid z > 0, r > 0, \theta \in (0, \pi)\}$ is invariant with respect to (4).

Proof. Note that $\dot{z}$ vanishes on the plane $\{z = 0\}$ and that $\dot{\theta}$ vanishes on $\{\theta = 0, \pi\}$. The uniqueness of solution of the initial value problem implies that any solution orbit cannot cross these planes. If $r = 0$, then $v = w = 0$ holds. However, since $w(0) = 0$ implies $w(t) = 0$ for any $t$, the solution with $r(0) > 0$ cannot touch on $r = 0$ in a finite time. 

It is easily seen that the following lemma holds (Figure 4 illustrates this lemma).

Lemma 3.6. The following statements hold:

(i) If $(z(0), r(0), \theta(0)) \in S$, then $\dot{\theta}(t)$ is negative for any $t > 0$.
(ii) If $z > 0$ and $\theta \in (\pi/2, \pi]$, then $\dot{z}$ is positive at $(z, r, \theta)$.
(iii) If $z > 0, \theta \in (\pi/2, \pi)$ and $r = \sqrt{\delta}$, then $\dot{r}$ is negative at $(z, r, \theta)$.
(iv) If $z > 0$ and $\theta \in [0, \pi/2)$, then $\dot{z}$ is negative at $(z, r, \theta)$.
(v) If $z > 0, 0 < r < \sqrt{\delta}, \theta \in [0, \pi/2)$, then $\dot{r}$ is positive at $(z, r, \theta)$.

Let us consider the solution of the initial value problem of (4) with the initial condition $(z(0), r(0), \theta(0)) = (z_0, r_0, \theta_0) \in S$ on the unstable manifold of the equilibrium $(0, \sqrt{\delta}, \theta_{-\infty})$. Since the unstable manifold of the equilibrium $(0, \sqrt{\delta}, \theta_{-\infty})$ is tangent to $E^u(\theta_{-\infty})$ appearing in Lemma 3.4, we can take $(z_0, r_0, \theta_0)$ so that

$z_0 > 0, \quad r_0 \in (0, \sqrt{\delta}), \quad \theta_0 \in (\pi/2, \pi)$.

Lemma 3.5 implies that $(z(t), r(t), \theta(t)) \in S$ for all $t > 0$. By Lemma 3.6(i), $\theta(t)$ is strictly monotone decreasing in $t > 0$. By Lemma 3.6(ii) and (iv), $z(t)$ is strictly
monotone increasing and $r(t) < \sqrt{\delta}$ as long as $\theta(t)$ is greater than $\pi/2$. Hence $\dot{\theta}$ is bounded from above by a negative constant:

$$\dot{\theta}(t) \leq -\frac{m_2 z_0}{\sqrt{\delta}} \sin \theta_0.$$ 

This implies that there exists $t_c > 0$ such that $\theta(t_c) = \pi/2$. Let $r_c = r(t_c), z(t_c) = z_c$. By Lemma 3.6(i), (iii), (v), the solution satisfies

$$0 < \theta(t) < \pi/2, \quad r(t) > r_c, \quad z(t) < z_c$$

for any $t > t_c$. The third statement of Main Theorem follows immediately from this fact and Lemma 3.3.

Since we have $\dot{\theta}(t) = -m_2 z/r_c < 0$, for a sufficiently small $\varepsilon > 0$ there exists $t_1$ such that $t_1 > t_c$ and $\theta(t_1) = \pi/2 - \varepsilon$. If $t > t_1$, then $\dot{z} \leq -(ar_c \cos(\pi/2 - \varepsilon))z$ and $z(t)$ exponentially decays as $t$ goes to infinity. Moreover, we obtain

$$\left( \delta - r^2 \right) r \leq \dot{r} \leq (\delta - r^2) r + m_2 z.$$ 

This implies that $r(t)$ converges to $\sqrt{\delta}$ as $t \to \infty$. Therefore there exists $\theta_{\infty} \in [0, \pi/2)$ such that $(z(t), r(t), \theta(t)) \to (0, \sqrt{\delta}, \theta_{\infty})$. This proves the first statement of the Main Theorem.

Next, we compare $\sin \theta_{-\infty}$ and $\sin \theta_{\infty}$. Recall that $\dot{z}(t) > 0$ for $t < t_c$ and $\dot{z}(t) < 0$ for $t > t_c$. This allows us to regard $z$ as a time-like variable in each time interval. By the chain rule we obtain

$$\frac{d\theta}{dz} = -\frac{m_2 z}{H(z) r^2} \tan \theta.$$ 

Also, $r$ can be seen as a function of $z$. Let $r_-(z)$ and $r_+(z)$ be parametrization of $r$ with respect to $z$ in $t < t_c$ and $t > t_c$, respectively. Similarly, let $\theta_-(z)$ and $\theta_+(z)$ be parametrization of $\theta(t)$ by $z$ in $t < t_c$ and $t > t_c$, respectively. We obtain

$$\int_{\theta_{-\infty}}^{\theta_{-\infty}} \frac{d\theta}{\tan \theta} = -m_2 \int_{0}^{z_c} \frac{zdz}{H(z)(r_-(z))^2}, \quad (14)$$

$$\int_{\theta_{\infty}}^{\theta_{\infty}} \frac{d\theta}{\tan \theta} = -m_2 \int_{0}^{z_c} \frac{zdz}{H(z)(r_+(z))^2}. \quad (15)$$

Figure 4. Direction field of $(r, z)$ and the curve $\{\dot{r} = 0\}$ at a fixed $\theta$. 
From (14) and (15) we obtain
\[
\sin \theta_\infty = \exp \left( m_2 \int_0^{z_c} \frac{z dz}{H(z)(r_-(z))^2} \right), \tag{16}
\]
\[
\sin \theta_{-\infty} = \exp \left( m_2 \int_0^{z_c} \frac{z dz}{H(z)(r_+(z))^2} \right). \tag{17}
\]

We prove the second statement of the Main Theorem by contradiction. Suppose that \(\sin \theta_{-\infty} \geq \sin \theta_\infty\) holds. It is necessary that
\[
\int_0^{z_c} \frac{z}{-H(z)} \left( \frac{1}{(r_-(z))^2} - \frac{1}{(r_+(z))^2} \right) dz \leq 0. \tag{18}
\]
Since we have \(\dot{r}(t_c) > 0, r_+(z) - r_-(z) \geq 0\) holds in a sufficiently small neighborhood of \(z = z_c\), where the equality holds only if \(z = z_c\). Therefore, as we have \(H(z) \leq -2z\), it is necessary for (18) that there exists \(z_+ \in (0, z_c)\) such that
\[
r_+(z_+) - r_-(z_+) = 0
\]
and
\[
\left. \frac{d}{dz} (r_+(z) - r_-(z)) \right|_{z = z_+} > 0. \tag{19}
\]
Otherwise, the left-hand side of (18) becomes positive. Let \(r_+ = r_+(z_+) = r_-(z_+)\). On the other hand, since we have \(H(z_+) < 0, r_+ < \sqrt{\delta}\) and \(\theta_-(z_+) > \pi/2 > \theta_+(z_+)\), we obtain
\[
\left. \frac{d}{dz} (r_+(z) - r_-(z)) \right|_{z = z_+} = \left( \frac{\delta - r_+^2}{H(z_+)} r_+ \cos \theta_+(z_+) \right) \frac{r_+}{r_+ \cos \theta_+(z_+)} - \left( \frac{\delta - r_+^2}{H(z_+)} r_+ \cos \theta_-(z_+) \right) \frac{1}{\cos \theta_+(z_+)} + \frac{1}{\cos \theta_-(z_+)}
\]
which is negative and contradicts (19). Thus \(\sin \theta_{-\infty} < \sin \theta_\infty\) must hold.

4. Relation between angles of incidence and reflection. In this section, the relationship between incidence and reflection is numerically investigated. Throughout this section, we set \(h(x) = (2x)^{-1/2}e^{-2x}\) and we do not necessarily assume \(m_0 = 0\).

For a prescribed angle of incidence \(\theta_{inc}\), we computed the angle of reflection \(\theta_{ref}\) in the following way. Let \(x_0\) be a positive number, which is a numerical parameter. We solved (1) with the initial data
\[
(x(0), y(0), v(0), w(0)) = \left( x_0, 0, -\sqrt{\delta} \cos \theta_{inc}, \sqrt{\delta} \sin \theta_{inc} \right)
\]
via DOP853 algorithm [5, §II.10] until \(x(t) > x_0\) and \(v(t) > 0\) are satisfied simultaneously, and computed \(\theta_{ref} = \arctan(|\dot{y}(t)/\dot{x}(t)|)\). Since \(h'(18.0) \approx 3.9 \times 10^{-17}\) is below machine epsilon for double precision, we may assume that \((\dot{x}(t), \dot{y}(t)) \approx (v(t), w(t))\) if \(x(t) > 18\). We chose \(x_0 = 20\) so that \(x_0 > 18\) holds.

Figure 5 presents \(F(\theta_{inc})\) and \(F'(\theta_{inc})\) for some parameter values. The numerical results suggest the following hypothesis.

**Hypothesis 1.** The function \(F: [0, \pi/2] \to [0, \pi/2]\) satisfies the following conditions:
\[
i) \ F(0) = 0 \text{ and } F(\pi/2) = \pi/2,
\]
\[ F(\theta) > \theta \text{ for any } \theta \in (0, \pi/2). \]

\[ F'(\theta) > 0 \text{ for any } \theta \in (0, \pi/2). \]

\[ F'(\pi/2) = 1. \]

Hypothesis 1 i) and ii) are true for \( m_0 = 0 \) from the Main Theorem. The conditions (i) and (iv) imply that \( F \) is written by

\[ F(\theta) = \theta + \theta(\pi - 2\theta)^2 g(\theta) \]  

for some function \( g \), provided that \( F \) is at least of class \( C^3 \). The smoothness of \( F \) should be proved in future studies. We approximate \( g \) by a polynomial

\[ q(\theta) = c_0 \theta^k + c_1 \theta^{k-1} + \cdots + c_k \]  

and approximate \( F \) by \( p(\theta) = \theta + \theta(\pi - 2\theta)^2 q(\theta) \). We estimated the coefficients \( c_0, c_1, \ldots, c_k \) from numerical data in the following way. There are some numerical parameters: the degree of polynomial \( k \), the number of data points \( N \), and the number of samples \( \tilde{N} \) for estimating the generalization error. Let \( \theta_n = n\pi/(2N) \) for \( n = 1, 2, \ldots, N-1 \). For each \( \theta_n \), we computed the angle of reflection \( \varphi_n = F(\theta_n) \) via the method mentioned above. Let \( \psi_n \) be

\[ \psi_n = \frac{\varphi_n - \theta_n}{\theta_n(\pi - 2\theta_n)^2}. \]

We applied the linear regression to \( \{(\theta_n, \psi_n)\}_{n=1}^{N-1} \) for estimating \( c_0, c_1, \ldots, c_k \). In addition, we estimated the generalization error: taking samples \( \tilde{\theta}_1, \tilde{\theta}_2, \ldots, \tilde{\theta}_{\tilde{N}} \) randomly from \( [0, \pi/2] \) and computing the reflection angle \( \tilde{\varphi}_n \) for \( n = 1, 2, \ldots, \tilde{N} \), we computed the root mean square error:

\[ E = \sqrt{\frac{1}{N} \sum_{n=1}^{\tilde{N}} (\psi_n - q(\tilde{\theta}_n))^2}. \]  

We applied these methods for various \( m_0 \) and \( \delta \) while \( m_2 = 1 \) was fixed. Figure 6 shows numerical results for \( k = 1 \) with \( E < 0.001 \). For these parameter values, there is a good agreement between \( F \) and a quartic function. \((c_0, c_1)\) moves away from the origin as \( \delta \) increases. As shown in Fig. 7(A), a larger \( \delta \) implies a larger \( E \). In fact, as seen in Fig. 7(B), the fitted curve with \( k = 1 \) is apparently different.
from the data obtained for \( m_0 = m_2 = 1 \) and \( \delta = 0.25 \). In such a case, we need to increase the degree of polynomial.

![Graph of \( (c_0, c_1) \) vs \( c_3 \) and \( \delta \) vs \( \sqrt{c_0^2 + c_1^2} \)](image)

**Figure 6.** The results of linear regression for (1) with \( m_2 = 1 \). Only the results satisfying \( E < 0.001 \) are plotted. (A) The estimated values of \( (c_0, c_1) \) for various \( \delta \) and \( m_0 \). (B) The dependence of \( \sqrt{c_0^2 + c_1^2} \) on \( \delta \). Red, blue, and green circles are results for \( m_0 = 0, 0.5, 1.0 \), respectively.

![Graph of \( \log_{10} E \) vs \( \delta \) and Numerical data of \( F(\theta_{\text{inc}}) \) for \( m_0 = m_2 = 1, \delta = 0.25 \) and fitted curve with \( k = 1 \) and \( k = 2 \).](image)

**Figure 7.** (A) \( \delta \) versus \( \log_{10} E \). The parameters are same as Fig. 6. (B) Numerical data of \( F(\theta_{\text{inc}}) \) for \( m_0 = m_2 = 1, \delta = 0.25 \) and fitted curve with \( k = 1 \) and \( k = 2 \).

5. **Concluding remarks: Billiards on square.** In this final section, we consider billiards on square of a particle which repeats motion in a straight-line and reflection from the boundary, where the particle collides with the boundary and the reflection angle is determined by \( \theta_{\text{ref}} = F(\theta_{\text{inc}}) \). This models the situation where the billiard table is so huge relative to the camphor size. Suppose that the billiard ball hits all the edges of a square \([0, 1] \times [0, 1]\) in turn as shown in Figure 8. Then the position of reflection and the angle of incidence are determined by iterations of \( \mathcal{R} : (x, \theta) \rightarrow (X(x, \theta), G(\theta)) \), where

\[
X(x, \theta) = (1 - x) \cot F(\theta), \quad G(\theta) = \frac{\pi}{2} - F(\theta).
\]  

This dynamical system makes sense as long as \( 0 < X(x, \theta) < 1 \) is satisfied. It should be noted that there is an ambiguity in the direction of motion.
The next theorem is concerned with a sufficient condition of the existence and stability of a square-shaped cycle. A necessary condition for the stability has been discussed in [10]. Although existence and stability of fixed point for $G$ have shown in [12, 16], it is worth stating here in a more general manner together with a proof.

**Theorem 5.1.** Suppose that $F \in C^1([0, \pi/2])$ is monotone increasing and satisfies $F(0) = 0$, $F(\pi/2) = \pi/2$, and $F(\theta) > \theta$ for $\theta \in (0, \pi/2)$. $R$ has the unique fixed point $(x^*, \theta^*)$ in $(0,1) \times (0,\pi/2)$ defined by

$$x^* = \frac{1}{1 + \tan F'(\theta^*)}$$

and $\theta^*$ is the fixed point of $G$. Accordingly, there exists a unique square-shaped periodic orbit. The linearized eigenvalues of $R$ at $(x^*, \theta^*)$ are $-\cot F'(\theta^*)$ and $-F''(\theta^*)$.

**Proof.** The intermediate value theorem and monotonicity of $F$ imply the unique existence of a fixed point of $G$. From $\tan \theta^* < \tan F(\theta^*)$ and $\tan G(\theta^*) = \tan \theta^*$, we obtain $0 < \theta^* < \pi/4 < F(\theta^*) < \pi/2$. Hence, $x^*$ given by (24) is included in the interval $(0,1)$. Since $G$ is independent of $x$, the eigenvalues of the linearized matrix of $R$ at the fixed point are its diagonal entries: $-\cot F'(\theta^*)$ and $-F''(\theta^*)$.

Since $\pi/4 < F'(\theta^*) < \pi/2$ holds, we have $| - \cot F'(\theta^*) | < 1$. Hence, the linear stability is determined by the eigenvalue $-F''(\theta^*)$.

We present two examples. The first example is concerned with the case where $F$ is quadratic. It is a generalization of [12] which studies the case where $a = 1/\pi$. It is important that the inequality $\theta_{\text{ref}} > \theta_{\text{inc}}$ alone is not sufficient for the stability of a limit cycle. In connection with the curve fitting results in the previous section, we consider the case where $F$ is a quartic function satisfying Hypothesis 1 as the second example. If $F$ is quartic, then a period-doubling bifurcation can occur. In [12], a period-doubling bifurcation was first observed numerically in the case where $F$ is cubic.

5.1. **Quadratic function.** Suppose that $F(\theta)$ is a quadratic function satisfying $F(0) = 0, F(\pi/2) = \pi/2, F(\theta) > \theta$ and $F'(\theta) > 0$ for $0 < \theta < \pi/2$. Then $F$ is given by

$$F(\theta) = \theta(1 + \pi a - 2a\theta),$$

where $0 < a \leq 1/\pi$. The theorem above implies the existence of a square-shaped cycle. Although it is easy to solve the fixed point equation $G(\theta) = \theta$ in this case, we do not need the closed-form solution to determine the stability. Indeed, $F''(\theta) =$
1 + πa − 4aθ is greater than 1 for any 0 < θ < π/4 if 0 < a ≤ 1/π. Therefore, the square-shaped cycle cannot be stable if F is quadratic. Furthermore, since we have

\[ G^2(θ) − θ = −a^2θ(π − 2θ) \left[ 4aθ^2 − 2(aπ + 2)θ + π \right], \]

there is no nontrivial periodic point of period 2. Accordingly, no parallel-piped orbit exists.

5.2. Quartic function. Based on the observation in the previous section, we suppose that F(θ) is a quartic function satisfying Hypothesis 1. We can write F by

\[ F(θ) = θ + θ(π − 2θ)^2(c_0θ + c_1), \]

which corresponds to the case where \( k = 1 \) in (21). From Hypothesis 1(i), (ii), (iv) we have

\((c_0 > 0) \land (c_1 = 0)\) ∨ \((πc_0 ≥ −2c_1) \land (c_1 ≥ 0)\).

Hypothesis (iii), the monotonicity of F, requires an additional assumption on \( c_0 \) and \( c_1 \). The theorem above implies the unique existence of a square-shaped cycle. This cycle can changes its stability depending on the parameter \( (c_0, c_1) \). Indeed, by solving the simultaneous equations

\[ G(θ) = θ, \quad F'(θ) = 1 \]

with respect to \( (c_0, c_1) \), we obtain a curve \{\( (c_0(θ), c_1(θ)) \mid 0 < θ < π/4 \}\},

\[ c_0(θ) = \frac{(π − 4θ)(π − 6θ)}{2θ^2(π − 2θ)^3}, \quad c_1(θ) = \frac{(π − 4θ)^2}{θ(π − 2θ)^3}, \]

(27)

on which the square-shaped cycle has the multiplier −1. It is an easy exercise to prove that a supercritical period-doubling bifurcation ([9, Chapter 4]) occurs when the parameter \( (c_0, c_1) \) crosses this curve transversally. A period-2 cycle, which corresponds to a parallel-piped orbit, appears from the period-doubling bifurcation. It should be noted that the period-doubling bifurcation curve is far from the parameter values estimated from the particle model in the previous section. This means that a period-doubling bifurcation of a square-shaped cycle does not occur in the particle model, provided that \( \delta \) is sufficiently small.

In Fig. 7(B), \( k = 2 \) fits the data better than \( k = 1 \). In this case, the function F is quintic and has three parameters \( c_0, c_1, \) and \( c_2 \). Since quartic functions are also included in this case, it is obvious that there exists a bifurcation surface of period-doubling bifurcations in \( (c_0, c_1, c_2) \)-space. It is, however, not amenable to further analysis by hand. More sophisticated and general methods are needed for understanding the dynamics and bifurcations of the discrete-time model.

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