Dynamical aspects of coupled dissipative gears were investigated numerically. We studied the transmissions of the rotational motions by coupled hard gears and those by coupled soft gears under a torque working on one of the gears. In particular, we considered the following two situations: P) the system contains a pair of gears, and T) the system contains three gears which form a regular triangle. If the system involves only hard gears which are coupled tightly, we obtain the trivial results that the transmissions of the rotational motions to other gears occur only in situation P). On the other hand, if the gears in the system are soft or coupled loosely, the transmissions of the rotational motions to other gears are observed only in situation T).

Our regular (macro) machines are usually constructed with tough components such as hard gears, shafts, bearings, etc. In such machines, these components need to be coupled tightly to realize their functions. Thus, they seem to be weak against some fluctuations. On the other hand in biological systems, several functions are realized by proteins which are generally soft and easy to deform. It is remarkable that they can work efficiently under the large influences of thermal fluctuations.

In this paper, we perform simulations of the systems consisting of hard gears or soft gears in order to directly compare the differences of the mechanical properties between our regular hard machines and soft machines in biological systems. First, we propose the ideal models of the coupled hard gears and the coupled soft gears. Second, we study the transmission properties of rotational motions using these systems in the following two situations: P) the system contains a pair of gears, and T) the system contains three gears where their rotational axes form a regular triangle (as in Figs. 1(c), (e) and (g)).

Now, a model of coupled gears is introduced. First, we propose the model of each individual gear as follows. We consider a group of particles which are connected to a common rotational axis by rigid rods with unit length and moving along the common circle in two dimensional space. If these particles interact repulsively, the form of this particles’ group becomes similar to that of our regular gears, where each rod indicates each tooth of the gear (as in Fig. 1(a)). Then, we regard the particles’ group as a model gear. By collecting a number of such model gears and fixing their rotational axes at a suitable interval, we obtain a model of the coupled gears as shown in Fig. 1. Here, the motion of each particle gives the motion of each tooth edge in gears. In this paper, we consider the cases with the over-damping limit.

The kinetic equation of each particle is given by

$$\dot{r}_j^i = - \sum_{(i,j) \neq (i',j')} C_{j,j'}^i \nabla_{r_j^i} V(|r_j^i - r_{j'}^{i'}|) + F_j^i. \quad (1)$$
Here, \( r_{ij} \) indicates a position of the \( j \)th particle in the \( i \)th gear in two dimensional space, and \( F_{ij} \) indicates the external torque working on the \( j \)th particle in the \( i \)th gear. Here, \(|r_{ij} - R_i| = 1\) always holds; \( R_i \) is the position of the rotational axis of the \( i \)th gear. This model belongs to a specific case of coupled phase oscillators.\(^3\)

In this paper, we employ \( V(r) = 1/r \) as the repulsive interaction potential between particles. \( C_{ij}^{i',j'} \) gives the magnitude of the repulsive force working between the \( j \)th particle in the \( i \)th gear and the \( j' \)th particle in the \( i' \)th gear. We set \( C_{ij}^{i',j'} = 1 \) for \( i \neq i' \) and \( C_{ij}^{i',j'} = A > 0 \) for \( i = i' \). Then, \( A \) is a parameter indicating the hardness of each gear. In this paper, we consider the case where each gear has four teeth (particles). Similar types of behavior to those reported in this paper may be observed if the number of teeth in each gear is larger.

Now, we study the motions of the coupled gears in two situations, P) and T). Here, the intervals between the rotational axes of gears (\(|R_i - R_{i'}|\)) are given as \( L \). For simplicity, we call the gears with \( i = 1, 2, 3 \) G1, G2, G3, respectively. In T), G1, G2 and G3 are arranged in the clockwise order. In the following, we show the transmissions of the rotational motions of this model when a torque works on one of the gears constantly in one direction.

Figures 1(b) and (c) show the typical temporal evolutions of the coupled hard gears (b) in P) and (c) in T) with \( A = 50 \) and \( L = 2 \), where a certain magnitude of the torque in the clockwise direction (+ direction), \( F \), works on G1 constantly (\( F_1^j = F, F_2^j = F_3^j = 0 \)). It is noted that only the periodic motions are observed as the dynamical motions of the system in the situations presented in this paper. In Fig. 1(b), both gears rotate in opposite directions. This means the rotational motion is transmitted from G1 to G2 in P). On the other hand in Fig. 1(c), only G1 rotates and each tooth in G2 or G3 only oscillates in a restricted area. Thus, the rotational motion is not transmitted from G1 to any other gears in T). These results seem consistent with our common belief.

Next, we focus on the behavior of the coupled soft gears. Figures 1(d) and (e) show the typical temporal evolutions of the coupled soft gears (d) in P) and (e) in T) under the same conditions as the previous except for the hardness of each gear (\( A = 2.6 \)). As shown in Fig. 1(d), the shapes of gears are drastically different from those in the hard gears systems because the teeth are pushed out from the area between gears by the repulsive forces between teeth (particles) belonging to different gears. Thus, two gears appear as if they are not engaged. Therefore, only G1 rotates in P) as in Fig. 1(d). This means the rotational motion is not transmitted to G2. On the other hand in T), with the certain \( |F| \),\(^4\) the rotational motion is transmitted from G1 to G2 as in Fig. 1(e), where G2 rotates in the \(-\) direction due to the + rotation of G1. In this case, each tooth in G3 oscillates in a restricted area. (Because of the symmetry, the rotational motion is transmitted from G1 to G3 if the torque in the \(+\) direction works on G1.)

The transmission of the rotational motions in T) is observed also in the case where each gear has sufficient hardness if \( L \) is appropriately large. Figures 1(f) and (g) show the typical temporal evolutions of the coupled hard (\( A = 50 \)) gears...
Coupled Gears

Fig. 1. (a) Illustration of a model gear. (b) ~ (g) Typical temporal evolutions of the system (from the upper to the lower) with (b) $A = 50$ and $L = 2$ in P), (c) $A = 50$ and $L = 2$ in T), (d) $A = 2.6$ and $L = 2$ in P), (e) $A = 2.6$ and $L = 2$ in T), (f) $A = 50$ and $L = 2.4$ in P) and (g) $A = 50$ and $L = 2.4$ in T). Dashed arrows indicate the direction of the torque $F$, and circles are just markers.

Fig. 2. (a)(b)(c) Force relations between gears. (d) Phase diagram of the system in T) for the transmissions of rotational motions by $F$ in the + direction.

(f) in P) and (g) in T) with $L = 2.4$. In these cases, each of the two gears does not sufficiently engage because the intervals between gears are so far apart that the couplings between them become loose. Thus, only G1 rotates in P) as in Fig. 1(f). On the other hand in T), with the certain $|F|$, the rotational motion is transmitted from G1 to G3 as shown in Fig. 1(g), where G3 rotates in the − direction due to the + rotation of G1. In this case, each tooth in G2 oscillates in a restricted area.
(Because of the symmetry, the rotational motion is transmitted from G1 to G2 if the torque in the − direction works on G1.)

Thus, we obtain the clear differences between the mechanical properties of the tightly coupled hard gears (with small $L$ and large $A$) and those of the other types of coupled gears. Next, we focus on the force balances between gears in T) to clarify the differences of the transmission mechanisms in several types of coupled gears.

Figure 2 shows the snap shots of the time evolution of (a) tightly coupled hard gears ($A = 50$ with $L = 2$), (b) loosely coupled hard gears ($A = 50$ with $L = 2.4$) and (c) coupled soft gears ($A = 2.6$ with $L = 2$) when a torque in the + direction works on G1 constantly. In Fig. 2(a), it is clear that the rotational directions of two teeth, tooth 1 in G2 and tooth 2 in G3, and the direction of the repulsive force working between these two teeth are close. Thus, G2 and G3 cannot rotate. On the other hand, with the increase of $L$, the rotational direction of the tooth 2 in G3 is distanced from the direction of the repulsive force between tooth 1 in G2 and tooth 2 in G3 as in Fig. 2(b). Thus, G3 can rotate in the − direction according to the + directional rotation of G1.

If each gear is soft, the following force relations are obtained, between teeth in three gears as in Fig. 2(c). I) Tooth 1 in G1 pushes tooth 2 in G3. II) Tooth 3 in G3, which is pushed by tooth 2 through two teeth between teeth 2 and 3, pushes tooth 4 in G2. III) Tooth 5 in G2, which is pushed by tooth 4 through two teeth between teeth 4 and 5, pushes tooth 6 in G1. IV) The force working between tooth 5 in G2 and tooth 6 in G1 does not interfere with the movement of tooth 5 in G2 but does with that of tooth 6 in G1. Here, fact I) induces fact II), and II) induces III). By facts III) and IV), tooth 5 in G2 moves to the inner area of the triangle, and after this, tooth 6 in G1 moves to this area. Then, G2 can also rotate due to the rotation of G1. Thus, the rotational motion is transmitted to G2 from G1 through G3 if the torque in the + direction works on G1.

Finally, we show the phase diagram for the transmission properties of coupled gears in T) against the + directional torque working on G1 as functions of $L$ and $A$ in Fig. 2(d). Here, the transmissions of the rotational motions from G1 to G3 like in Fig. 1(g) occur in the region with dashed strips, and those from G1 to G2 like in Fig. 1(e) occur in the region with solid strips. As shown in this diagram, the transmissions of the rotational motions occur in a certain range of $L$ if $A$ is large enough. On the other hand, the transmissions of the rotational motions occur in a wide range of $L$ if each gear is appropriately soft.

In this paper, we investigated the transmissions of the rotational motions by the hard gears and those by the soft gears, and obtained many different transmission properties from these systems. These results seem to provide important hints for understanding the mechanisms of several functions in molecular machines.

References

4) A. Awazu, preprint.