velocity of particles i and j as a vector sum of their components parallel and perpendicular to the unit vector $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$. We write the velocity of particle i as

$$\mathbf{v}_i = \mathbf{v}_{i,\parallel} + \mathbf{v}_{i,\perp}, \tag{8.23}$$

where $\mathbf{v}_{i,\parallel} = (\mathbf{v}_i \cdot \hat{\mathbf{r}}_{ij})\hat{\mathbf{r}}_{ij}$, and

$$\mathbf{v}'_{i,\parallel} = \mathbf{v}_{j,\parallel} \qquad \mathbf{v}'_{j,\parallel} = \mathbf{v}_{i,\parallel} \tag{8.24a}$$

$$\mathbf{v}'_{i,\perp} = \mathbf{v}_{i,\perp} \qquad \mathbf{v}'_{j,\perp} = \mathbf{v}_{j,\perp}. \tag{8.24b}$$

Hence, we can write $\mathbf{v}'_i$ as

$$\begin{aligned}\mathbf{v}'_i &= \mathbf{v}'_{i,\parallel} + \mathbf{v}'_{i,\perp} = \mathbf{v}_{j,\parallel} + \mathbf{v}_{i,\perp} \\ &= \mathbf{v}_{j,\parallel} - \mathbf{v}_{i,\parallel} + \mathbf{v}_{i,\parallel} + \mathbf{v}_{i,\perp} \\ &= [(\mathbf{v}_j - \mathbf{v}_i) \cdot \hat{\mathbf{r}}_{ij}]\,\hat{\mathbf{r}}_{ij} + \mathbf{v}_i.\end{aligned} \tag{8.25}$$

The change in the velocity of particle i at a collision is given by

$$\Delta\mathbf{v}_i = \mathbf{v}'_i - \mathbf{v}_i = -[(\mathbf{v}_i - \mathbf{v}_j) \cdot \hat{\mathbf{r}}_{ij}]\hat{\mathbf{r}}_{ij}, \tag{8.26}$$

or

$$\Delta\mathbf{v}_i = -\Delta\mathbf{v}_j = \left(\frac{\mathbf{r}_{ij}\, b_{ij}}{\sigma^2}\right)_{\text{contact}}, \tag{8.27}$$

where $b_{ij} = \mathbf{v}_{ij} \cdot \mathbf{r}_{ij}$, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, and we have used the fact that $|\mathbf{r}_{ij}| = \sigma$ at contact.

Exercise 8.14 Velocity distribution of hard rods
Use (8.20) and (8.21) to show that $v'_i = v_j$ and $v'_j = v_i$ in one dimension; that is, two colliding hard rods of equal mass exchange velocities. If you start a system of hard rods with velocities chosen from a uniform random distribution, will the velocity distribution approach the equilibrium Maxwell–Boltzmann distribution? ■

We now consider the criteria for a collision to occur. Consider disks i and j at positions $\mathbf{r}_i$ and $\mathbf{r}_j$ at $t = 0$. If they collide at a time t_{ij} later, their centers will be separated by a distance σ:

$$|\mathbf{r}_i(t_{ij}) - \mathbf{r}_j(t_{ij})| = \sigma. \tag{8.28}$$

During the time t_{ij}, the disks move with constant velocities. Hence, we have

$$\mathbf{r}_i(t_{ij}) = \mathbf{r}_i(0) + \mathbf{v}_i(0)\, t_{ij}, \tag{8.29}$$

and

$$\mathbf{r}_j(t_{ij}) = \mathbf{r}_2(0) + \mathbf{v}_2(0)\, t_{ij}. \tag{8.30}$$

If we substitute (8.29) and (8.30) into (8.28), we find

$$[\mathbf{r}_{ij} + \mathbf{v}_{ij} t_{ij}]^2 = \sigma^2, \tag{8.31}$$

where $\mathbf{r}_{ij} = \mathbf{r}_i(0) - \mathbf{r}_j(0)$, $\mathbf{v}_{ij} = \mathbf{v}_i(0) - \mathbf{v}_j(0)$, and

$$t_{ij} = \frac{-\mathbf{v}_{ij} \cdot \mathbf{r}_{ij} \pm \sqrt{(\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})^2 - v_{ij}^2(r_{ij}^2 - \sigma^2)}}{v_{ij}^2}. \tag{8.32}$$

Because $t_{ij} > 0$ for a collision to occur, we see from (8.32) that the condition

$$\mathbf{v}_{ij} \cdot \mathbf{r}_{ij} < 0, \tag{8.33}$$

must be satisfied. That is, if $\mathbf{v}_{ij} \cdot \mathbf{r}_{ij} > 0$, the particles are moving away from each other and there is no possibility of a collision.

If the condition (8.33) is satisfied, then the discriminant in (8.32) must satisfy the condition

$$(\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})^2 - v_{ij}^2(r_{ij}^2 - \sigma^2) \geq 0. \tag{8.34}$$

If the condition (8.34) is satisfied, then the quadratic in (8.32) has two roots. The smaller root corresponds to the physically significant collision because the disks are impenetrable. Hence, the physically significant solution for the time of a collision t_{ij} for particles i and j is given by

$$t_{ij} = \frac{-b_{ij} - [b_{ij}^2 - v_{ij}^2\,(r_{ij}^2 - \sigma^2)]^{1/2}}{v_{ij}^2}. \tag{8.35}$$

Exercise 8.15 Calculation of collision times
Write a short program that determines the collision times (if any) of the following pairs of particles. It would be a good idea to draw the trajectories to confirm your results. Consider the cases: $\mathbf{r}_1 = (2, 1)$, $\mathbf{v}_1 = (-1, -2)$, $\mathbf{r}_2 = (1, 3)$, $\mathbf{v}_2 = (1, 1)$; $\mathbf{r}_1 = (4, 3)$, $\mathbf{v}_1 = (2, -3)$, $\mathbf{r}_2 = (3, 1)$, $\mathbf{v}_2 = (-1, -1)$; and $\mathbf{r}_1 = (4, 2)$, $\mathbf{v}_1 = (-2, \frac{1}{2})$, $\mathbf{r}_2 = (3, 1)$, $\mathbf{v}_2 = (-1, 1)$. As usual, choose units so that $\sigma = 1$. ■

Our hard disk program implements the following steps. We first find the collision times and the collision partners for all pairs of particles i and j. We then do the following.

1. Locate the minimum collision time $t_{\min}$;
2. Advance all particles using a straight line trajectory until the collision occurs; that is, displace particle i by $\mathbf{v}_i\, t_{\min}$ and update its next collision time;
3. Compute the postcollision velocities of the colliding pair `nextCollider` and `nextPartner`;
4. Calculate the physical quantities of interest and accumulate data;
5. Update the collision partners of the colliding pair, `nextCollider` and `nextPartner`, and all other particles that were to collide with either `nextCollider` or `nextPartner` if `nextCollider` and `nextPartner` had not collided first;
6. Repeat steps 1–5 indefinitely.

Methods for carrying out these steps are listed in the following: