Temps de collision externe entre les particules

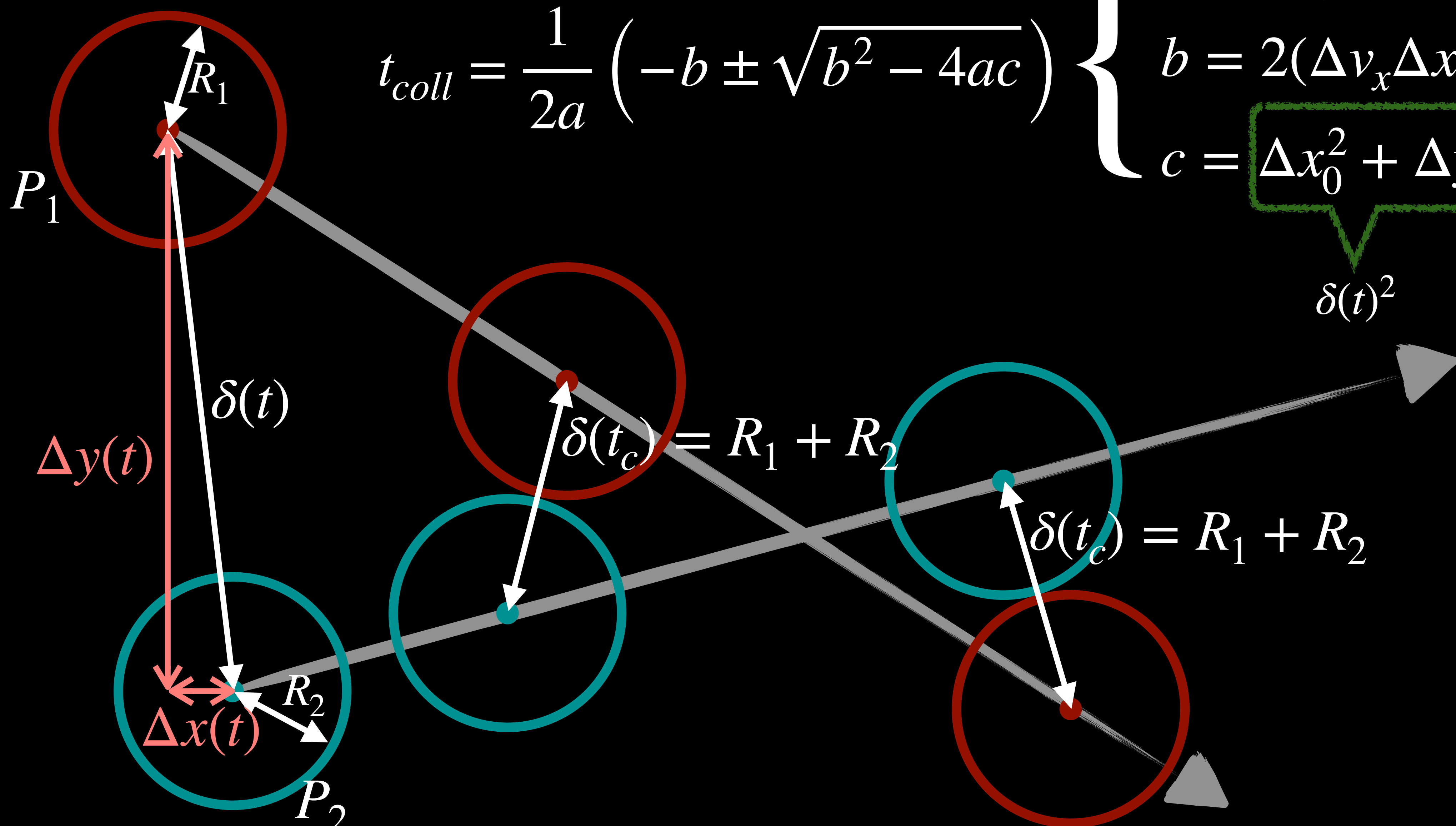
$$\left.\begin{aligned}\vec{r}_1(t) &= \vec{r}_1(0) + \vec{v}_1 t \\ \vec{r}_2(t) &= \vec{r}_2(0) + \vec{v}_2 t\end{aligned}\right\} \quad \delta(t) = \sqrt{\Delta x(t)^2 + \Delta y(t)^2}$$

$$\Delta x(t) = x_1(t) - x_2(t)$$

$$\Delta y(t) = y_1(t) - y_2(t)$$

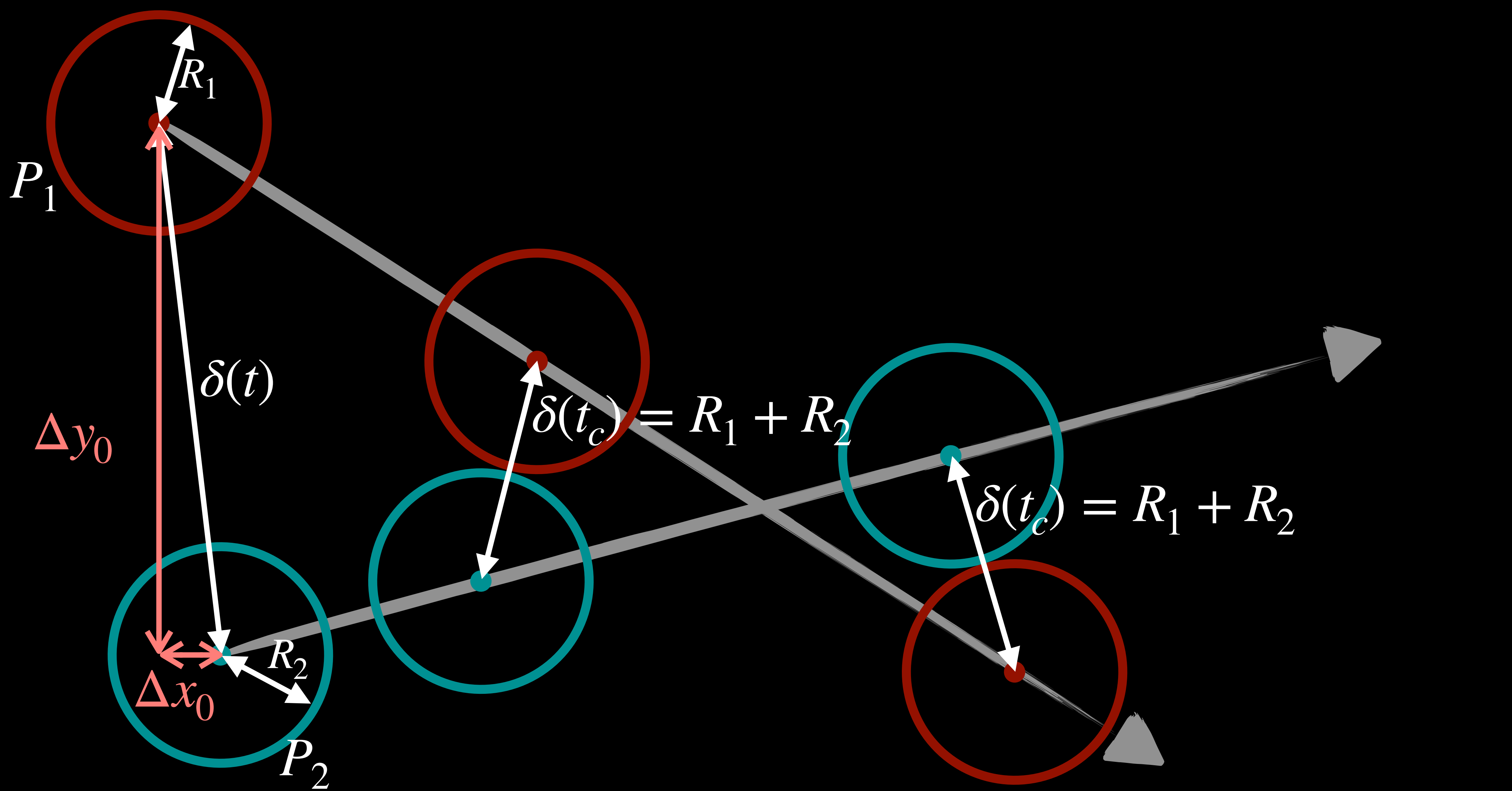
Condition pour une collision externe: $\delta(t_{coll}) = R_1 + R_2$ $\quad \boxed{(R_1 + R_2)^2 = \Delta x(t_c)^2 + \Delta y(t_c)^2}$

$$t_{coll} = \frac{1}{2a}\left(-b \pm \sqrt{b^2 - 4ac}\right) \quad \begin{cases} a = \Delta v_y^2 + \Delta v_x^2 \quad > 0 \\ b = 2(\Delta v_x \Delta x_0 + \Delta v_y \Delta y_0) \\ c = \underbrace{\Delta x_0^2 + \Delta y_0^2}_{\delta(t)^2} - \underbrace{\left(R_1 + R_2\right)^2}_{\delta(t_{coll})^2} > 0 \end{cases}$$



Temps de collision externe entre les particules

$$t_{coll} = \frac{1}{2a}\left(-b \pm \sqrt{\overbrace{b^2 - \underbrace{4ac}_{>0}}^{\Omega > 0}}\right) \quad \begin{cases} a = \Delta v_y^2 + \Delta v_x^2 \quad > 0 \\ b = 2(\Delta v_x \Delta x_0 + \Delta v_y \Delta y_0) \\ c = \Delta x_0^2 + \Delta y_0^2 - (R_1 + R_2)^2 \ > 0 \end{cases}$$



Temps de collision externe entre les particules

$\Omega > 0$

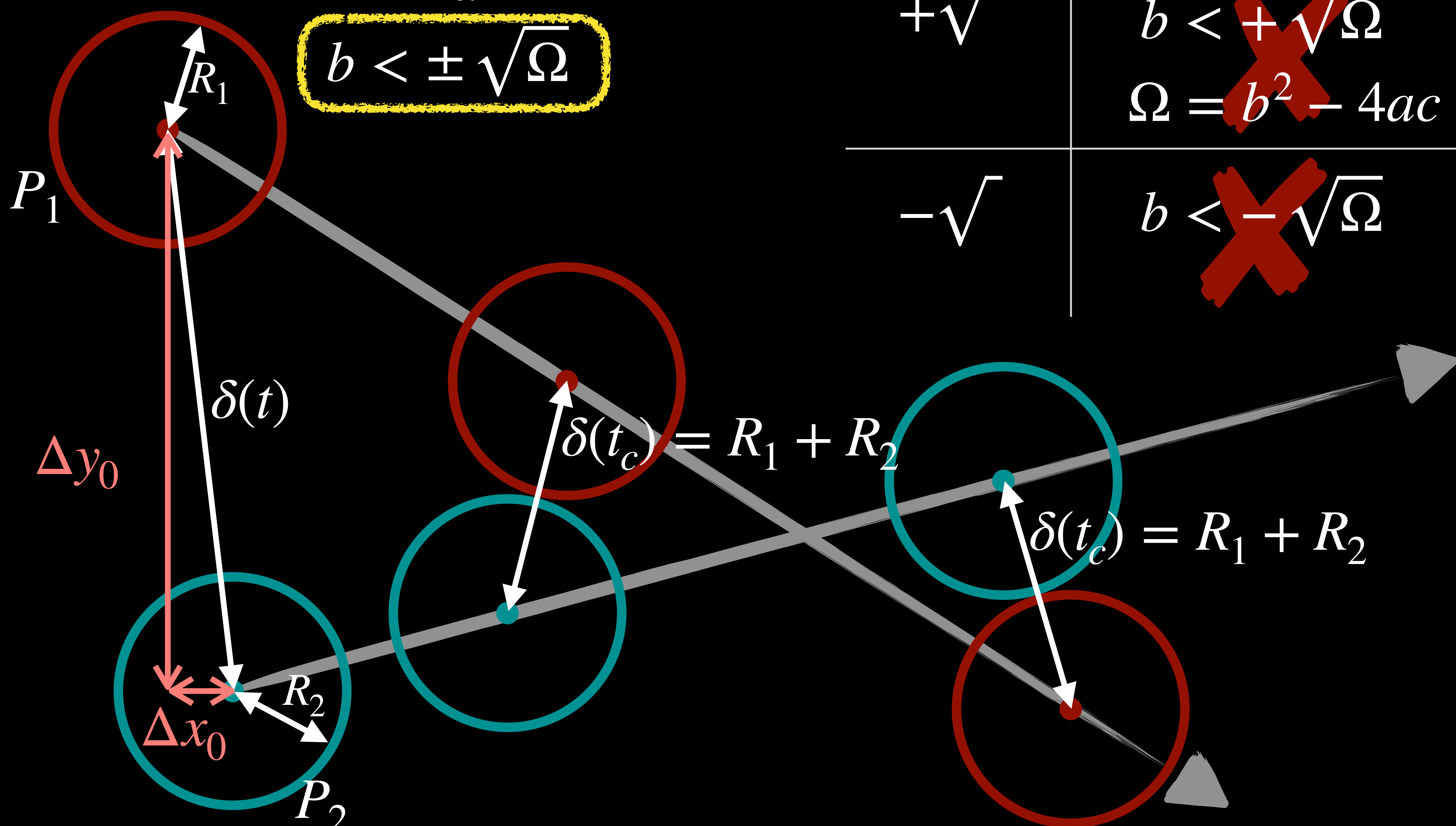
$$t_{coll} = \frac{1}{2a}\left(-b \pm \sqrt{\underbrace{b^2 - 4ac}_{>0}}\right) \quad \begin{cases} a = \Delta v_y^2 + \Delta v_x^2 & > 0 \\ b = 2(\Delta v_x \Delta x_0 + \Delta v_y \Delta y_0) \\ c = \Delta x_0^2 + \Delta y_0^2 - (R_1 + R_2)^2 & > 0 \end{cases}$$

Question : $0 < t_{coll}$

$$0 < \frac{1}{2a}\left(-b \pm \sqrt{\Omega}\right)$$

$$\boxed{b < \pm\sqrt{\Omega}}$$

	$b > 0$	$b < 0$
$+\sqrt{}$	$\cancel{b < +\sqrt{\Omega}}$ $\cancel{\Omega = b^2 - 4ac}$	$-\lvert b\rvert < +\sqrt{\Omega}$ ✓
$-\sqrt{}$	$\cancel{b < -\sqrt{\Omega}}$	$-\lvert b\rvert < -\sqrt{\Omega}$ $b^2 < \Omega$ ✓ $0 < 4ac$



Temps de collision externe entre les particules

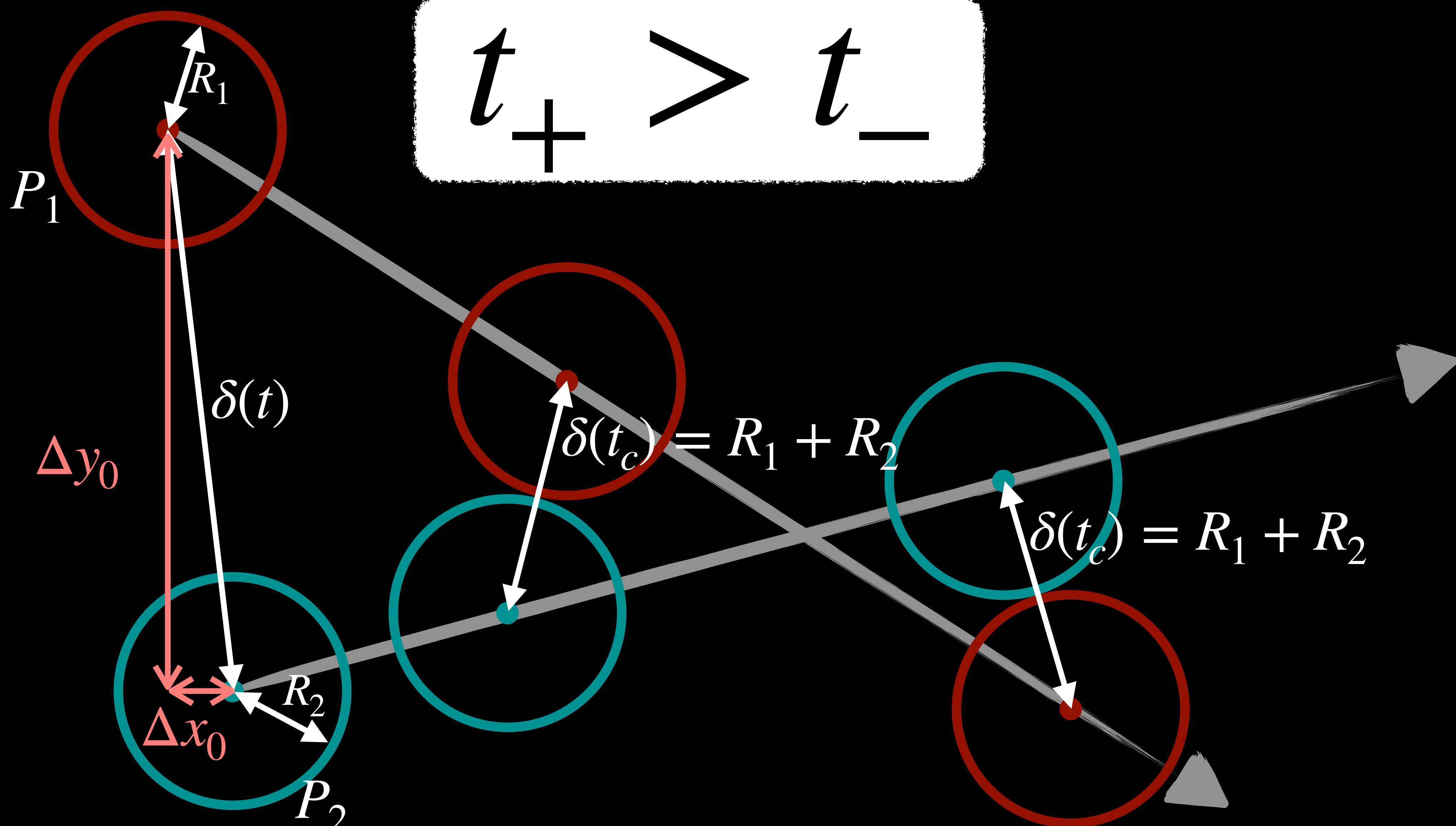
$$t_+, t_- > 0$$

$$t_+ = \frac{1}{2a}\left(-b + \sqrt{\Omega}\right)$$

$$t_- = \frac{1}{2a}\left(-b - \sqrt{\Omega}\right)$$

$$\begin{cases} a = \Delta v_y^2 + \Delta v_x^2 \\ b = 2(\Delta v_x \Delta x_0 + \Delta v_y \Delta y_0) \quad < 0 \quad ① \\ c = \Delta x_0^2 + \Delta y_0^2 - (R_1 + R_2)^2 \\ \Omega = b^2 - 4ac \quad > 0 \quad ② \end{cases}$$

$$\boxed{t_+ > t_-}$$



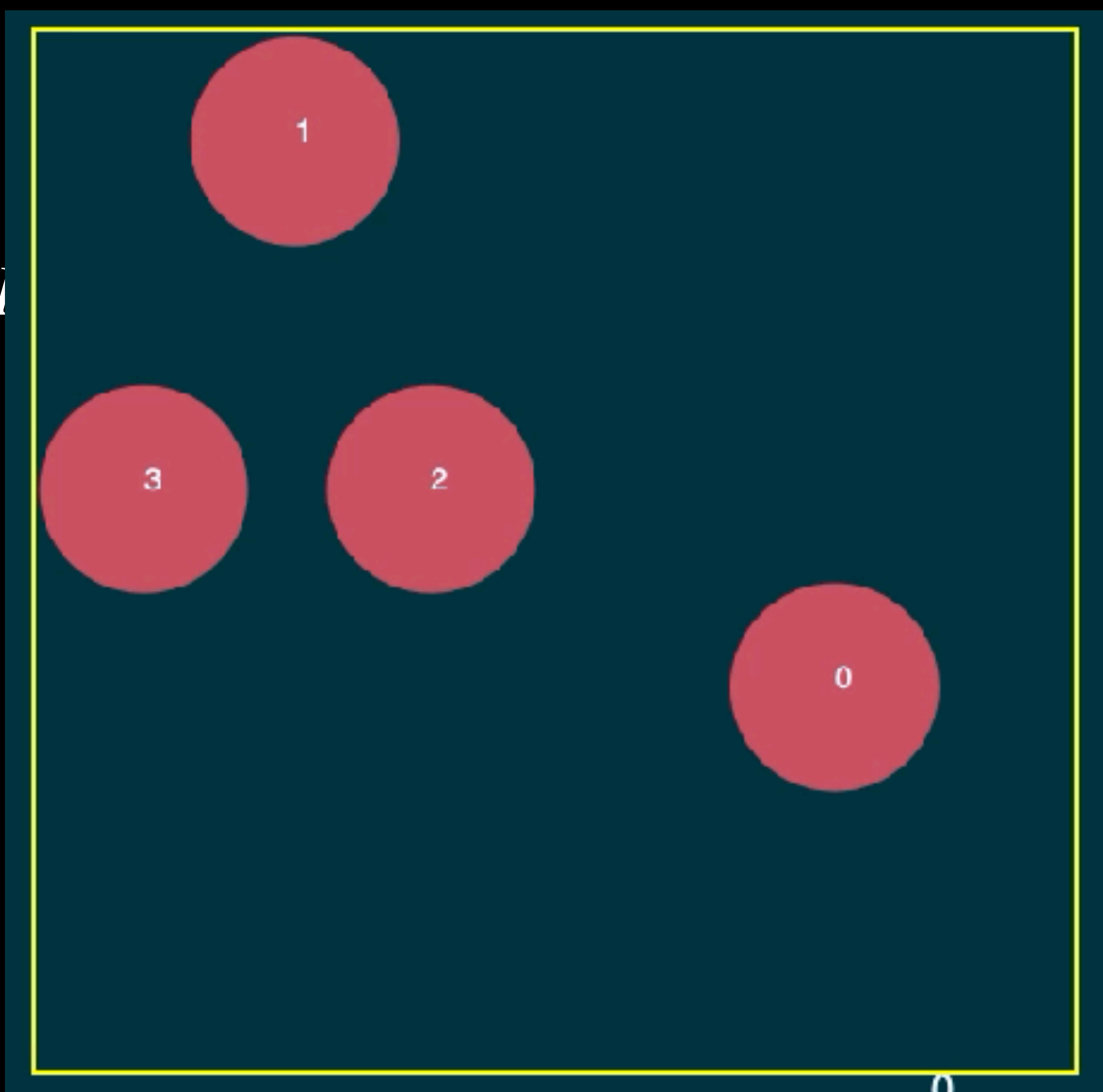
Temps de collision externe entre les particules

$$t_+, t_- > 0$$

$$t_+ = \frac{1}{2a}\left(-b + \sqrt{\Omega}\right)$$

$$t_- = \frac{1}{2a}\left(-b - \sqrt{\Omega}\right)$$

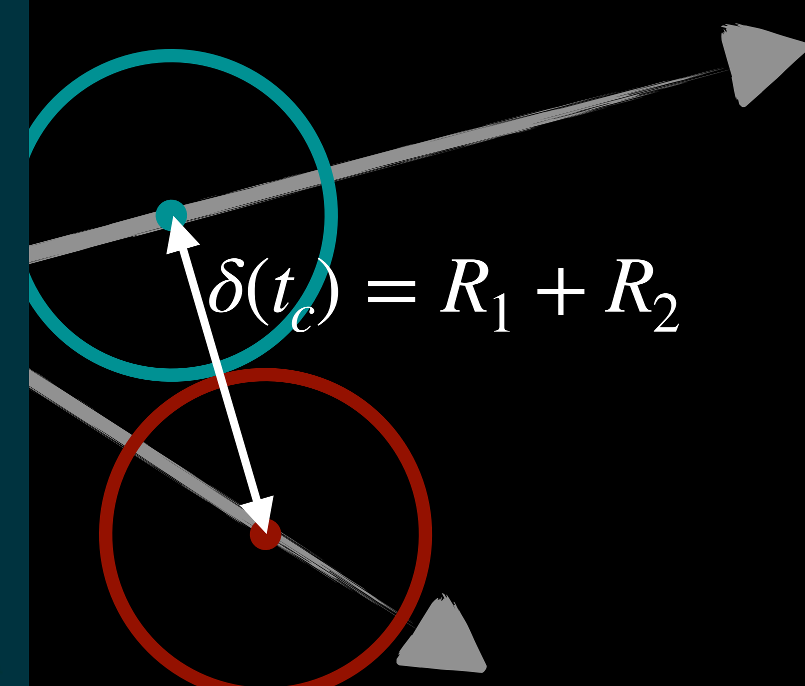
$$\begin{cases} a = \Delta v_y^2 + \Delta v_x^2 \\ b = 2(\Delta v_x \Delta x_0 + \Delta v_y \Delta y_0) \quad < 0 \quad \textbf{1} \\ c = \Delta x_0^2 + \Delta y_0^2 - (R_1 + R_2)^2 \\ \Omega = b^2 - 4ac \quad > 0 \quad \textbf{2} \end{cases}$$




```
dx = p[i_1].x - p[i_2].x
dy = p[i_1].y - p[i_2].y

dvx = p[i_1].vx - p[i_2].vx
dvy = p[i_1].vy - p[i_2].vy

A = …, B = …, C = …, Omega = …
```



Temps de collision externe entre les particules

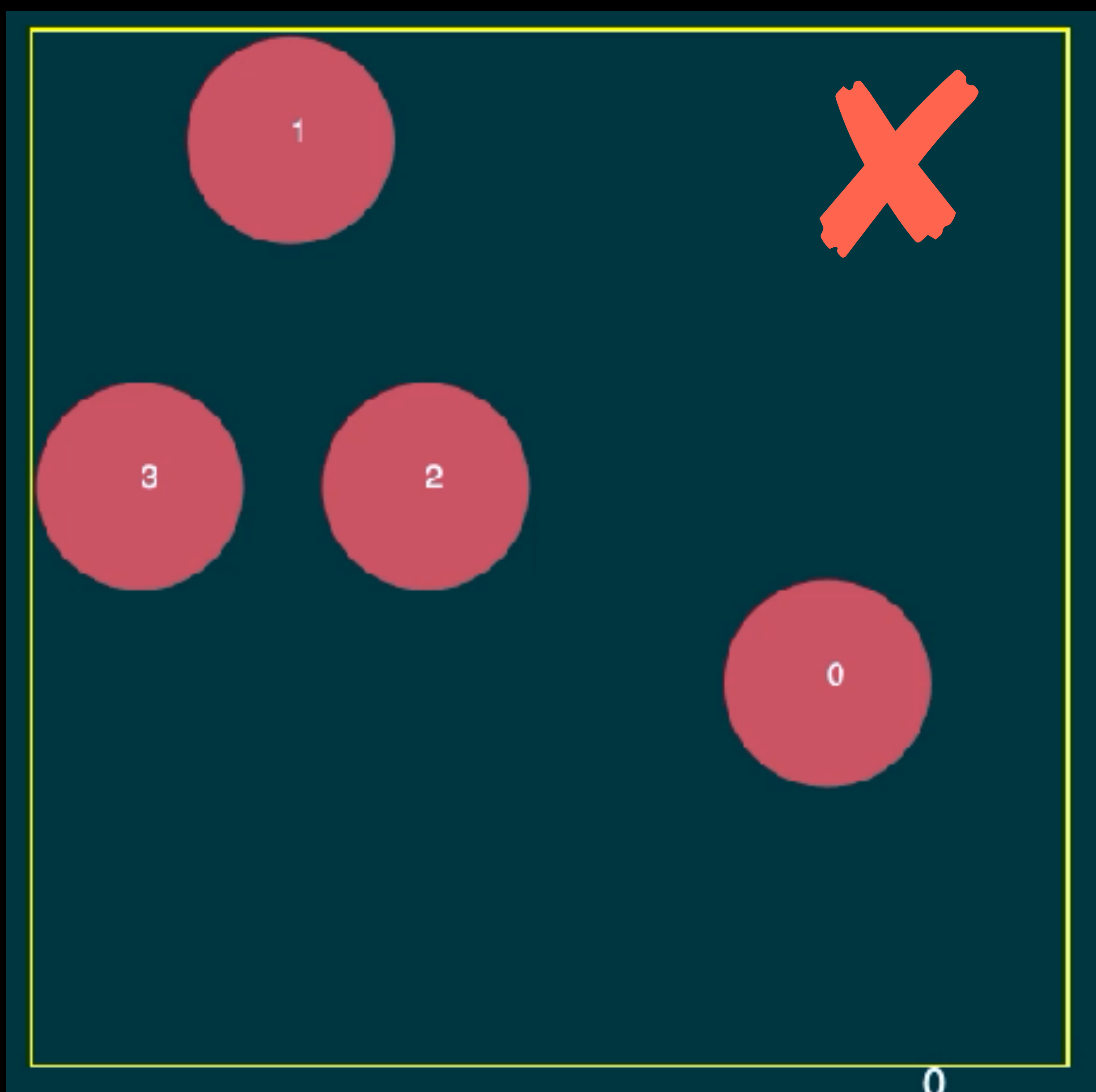
$$t_{coll} = \frac{1}{2a}\left(-b \pm \sqrt{b^2 - 4ac}\right)$$

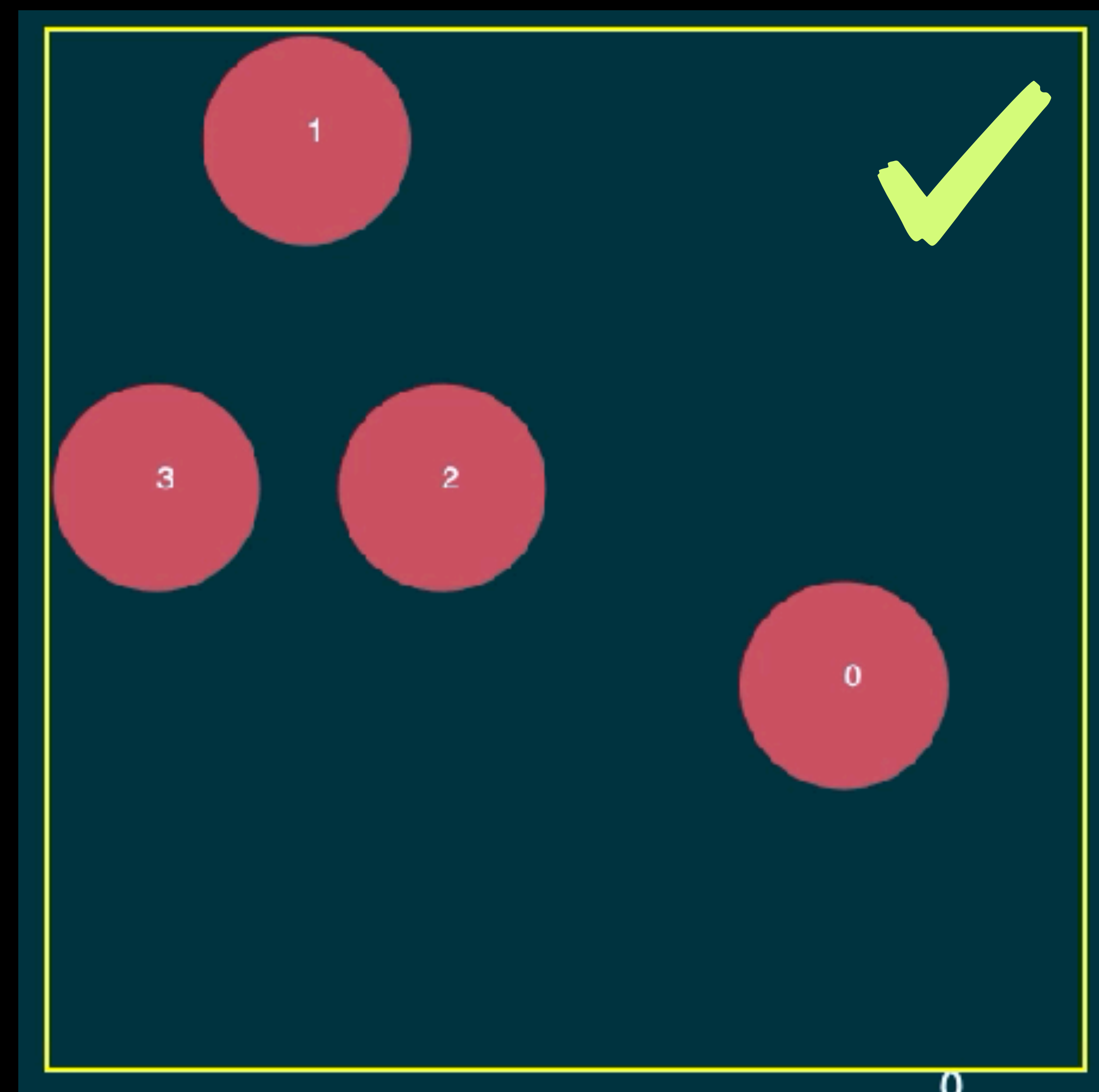
! $\Omega > 0$

$$t_{coll} = \frac{1}{2a}\left(-b - \sqrt{b^2 - 4ac}\right)$$

1 $b < 0$

2 $\Omega > 0$





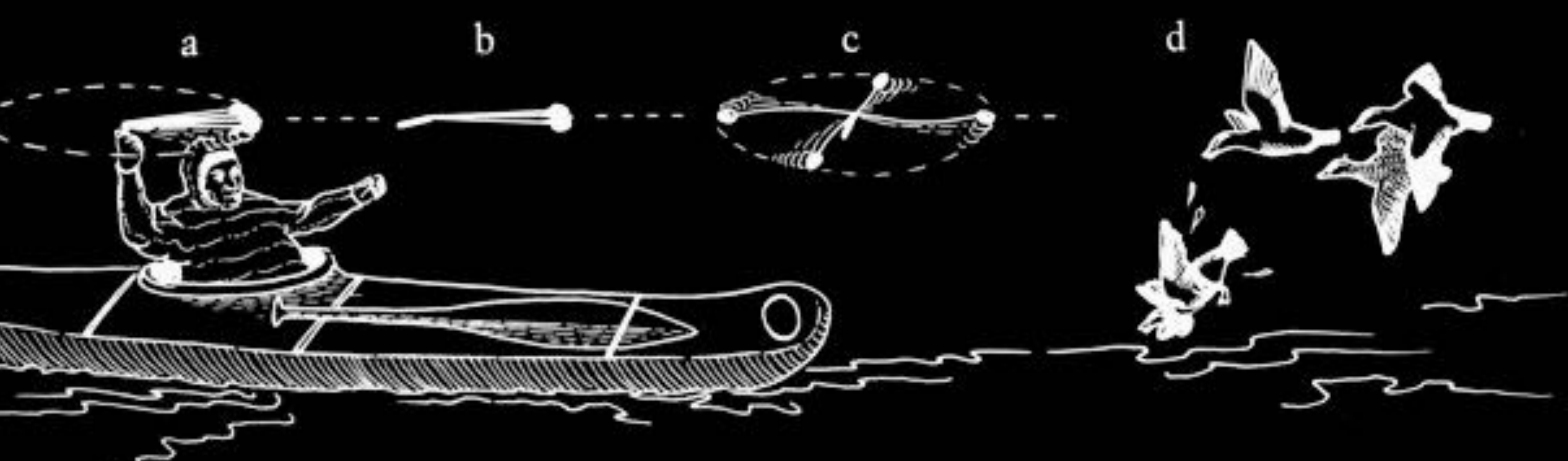
Temps de collision entre les particules

Collision intern

$$t_{coll} = \frac{1}{2a}\left(-b + \sqrt{b^2 - 4ac}\right)$$

1 $c < 0$

2 $\Omega > 0$



From Inua: Spirit World of the Bering Sea Eskimo by William W. Fitzhugh and Susan A. Kaplan, 1982, fig. 52.

Temps de collision entre les particules

Collision intern

$$t_{coll} = \frac{1}{2a}\left(-b + \sqrt{b^2 - 4ac}\right)$$

1 $c < 0$

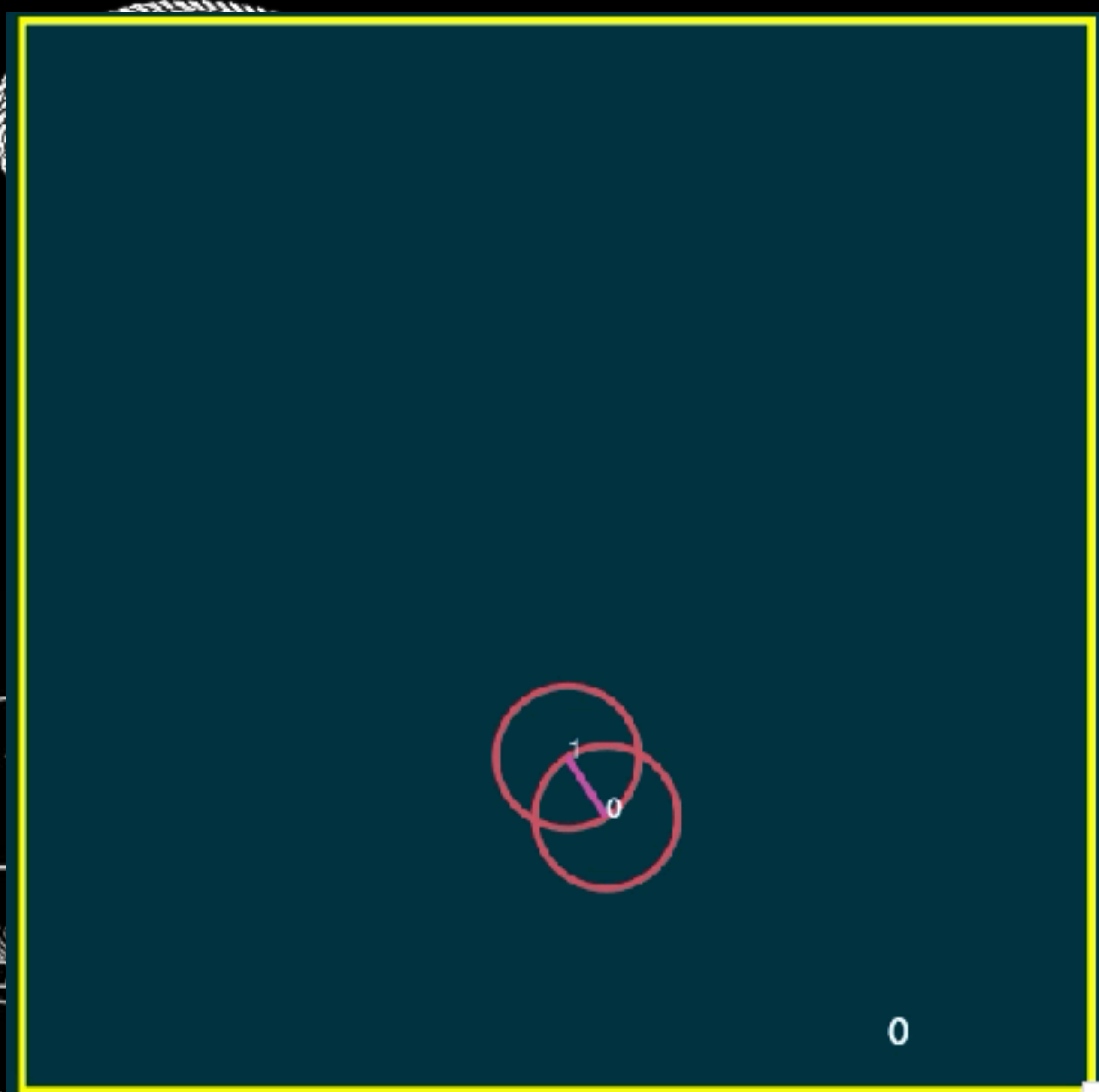
2 $\Omega > 0$

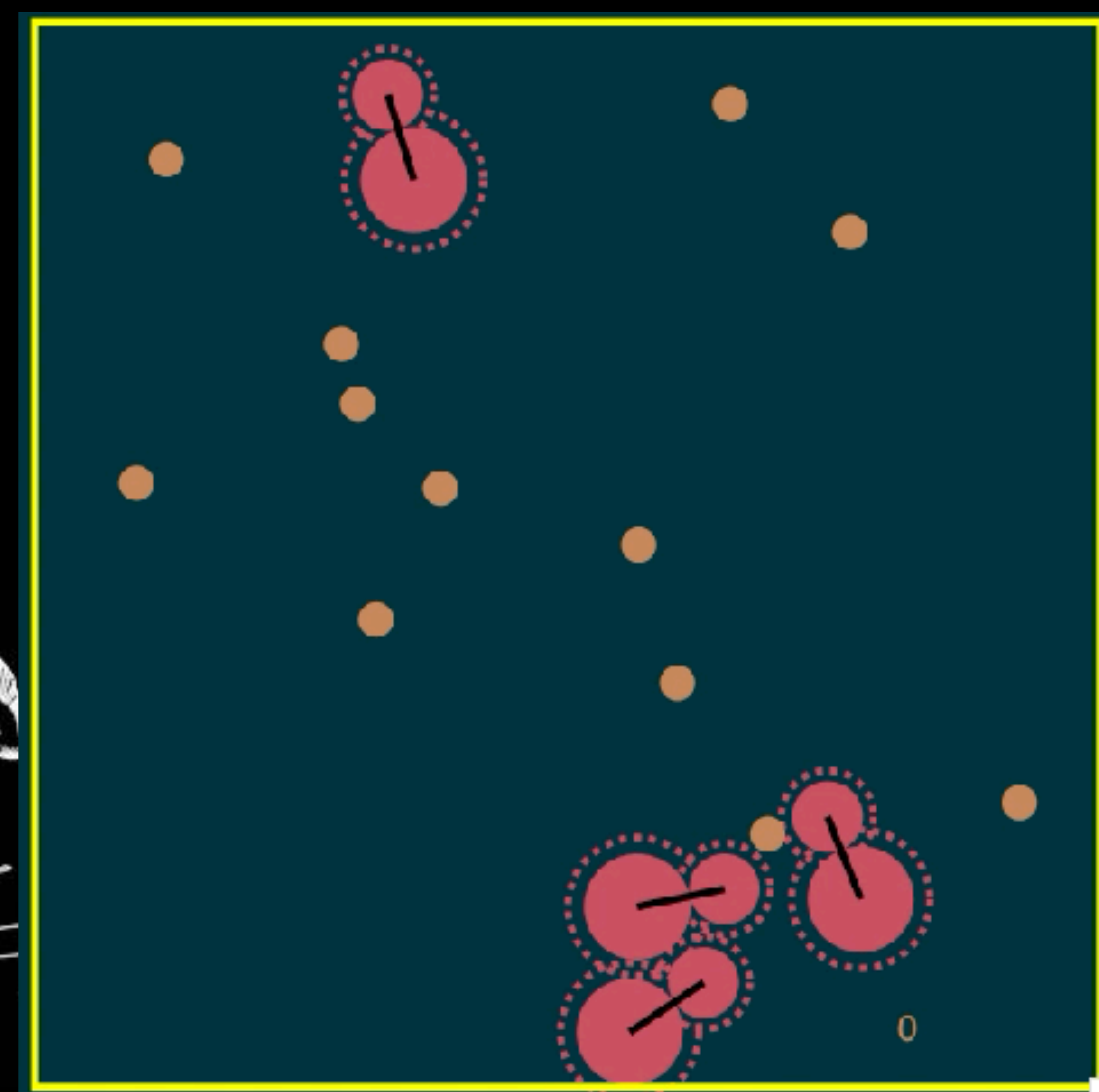
Collision externe

$$t_{coll} = \frac{1}{2a}\left(-b - \sqrt{b^2 - 4ac}\right)$$

1 $b < 0$

2 $\Omega > 0$





Fr[illegible]
Fitzhugh and Susan A. Kaplan, 1982, fig. 52.

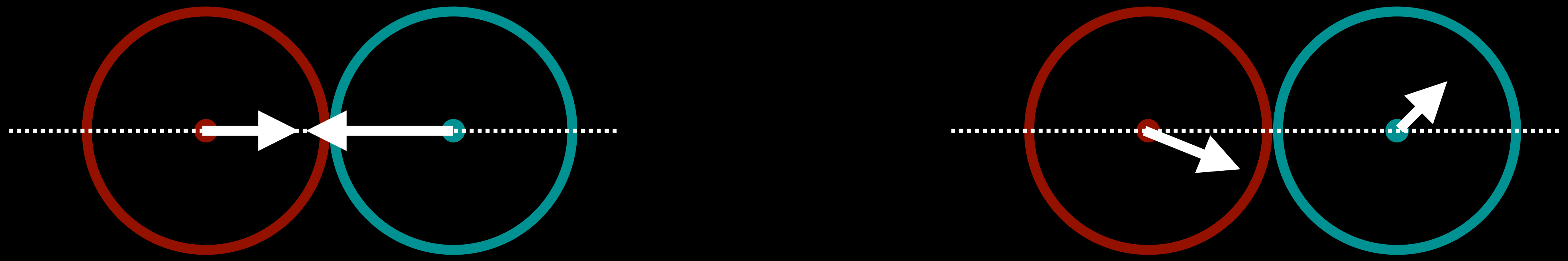
Mise à jour de la vitesse après la collision

$$E = \frac{1}{2}\sum_{i=1}^{N} m_i \overrightarrow{v}_i^2 = const \quad \text{(1)} \qquad \overrightarrow{F} = \sum_i^N \overrightarrow{F}_i = \sum_i^N \dot{\overrightarrow{p}}_i = 0 \quad \text{(2)}$$

(1) ⇒

$$m_1\left(\overrightarrow{v}_1\right)^2 + m_2\left(\overrightarrow{v}_2\right)^2 = m_1\left(\overrightarrow{v}'_1\right)^2 + m_2\left(\overrightarrow{v}'_2\right)^2$$

(2) ⇒ $m_1\overrightarrow{v}_1 + m_2\overrightarrow{v}_2 = m_1\overrightarrow{v}'_1 + m_2\overrightarrow{v}'_2$

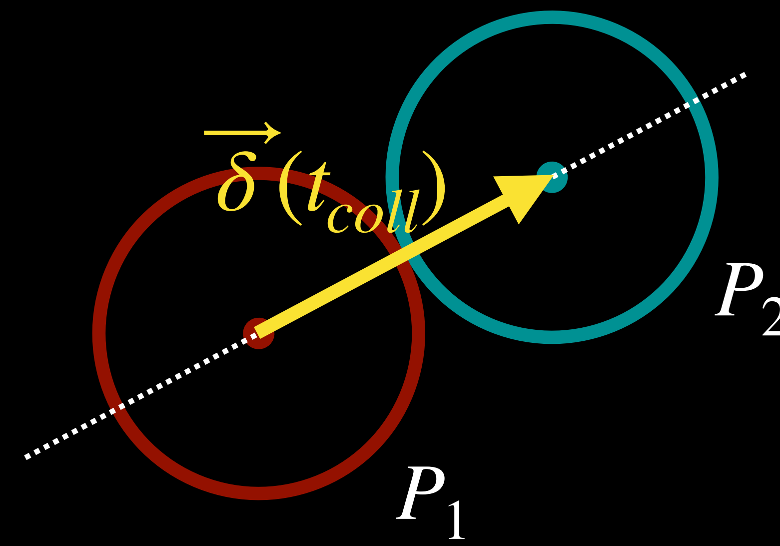


Mise à jour de la vitesse après la collision

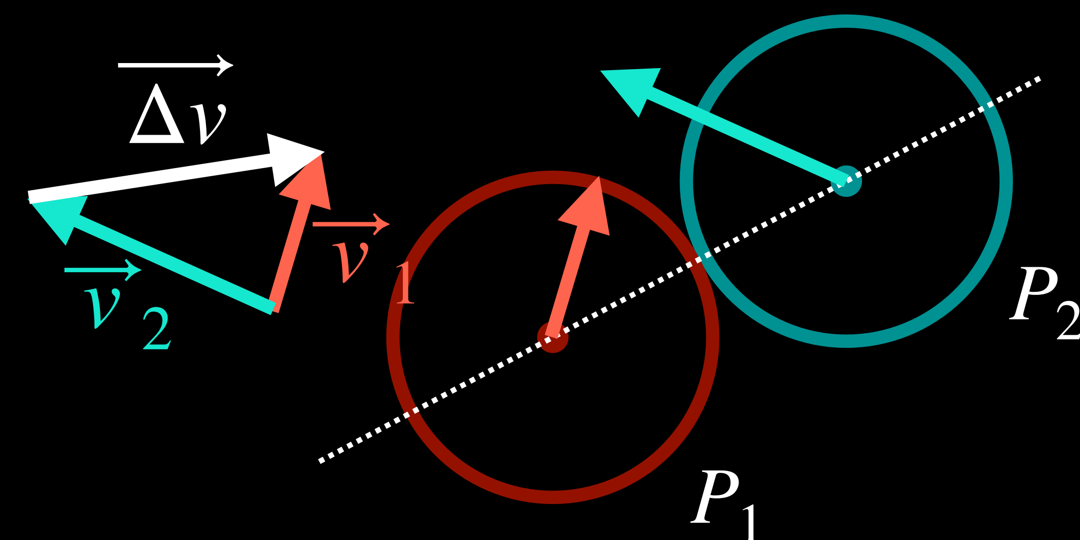
$$\vec{\delta}(t_{coll}) = \vec{r_2}(t_{coll}) - \vec{r_1}(t_{coll})$$

$$\widehat{\vec{\delta}}(t_{coll}) = \frac{\vec{\delta}}{|\vec{\delta}|} \qquad |\vec{\delta}| = \sqrt{\delta_x^2 + \delta_y^2}$$

$$= \cancel{R_1 + R_2}$$



$$\overrightarrow{\Delta v} = \vec{v}_1 - \vec{v}_2$$



$$\boxed{\begin{aligned}\vec{v}'_1 &= \vec{v}_1 - \frac{2m_2}{m_1+m_2}\left(\widehat{\vec{\delta}} \cdot \overrightarrow{\Delta v}\right)\widehat{\vec{\delta}} \\ \vec{v}'_2 &= \vec{v}_2 + \frac{2m_1}{m_1+m_2}\left(\widehat{\vec{\delta}} \cdot \overrightarrow{\Delta v}\right)\widehat{\vec{\delta}}\end{aligned}}$$

https://williamecraver.wixsite.com/elastic-equations

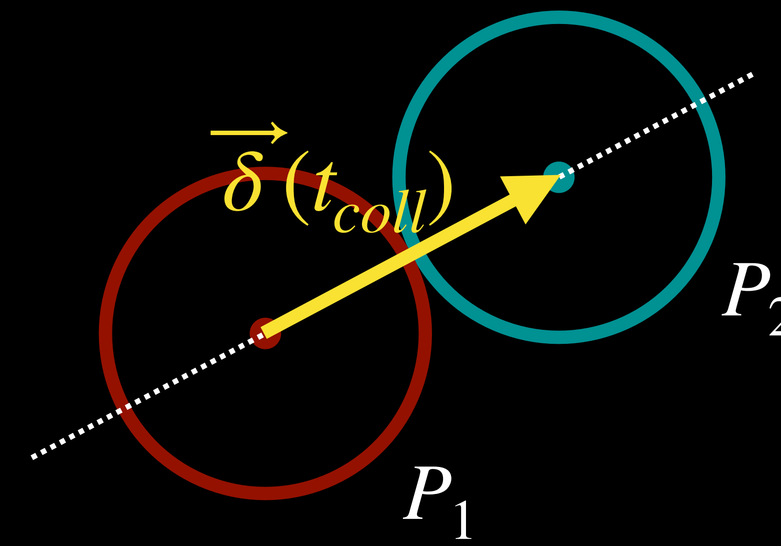
```
dx = p[i_2].x - p[i_1].x
dy = p[i_2].y - p[i_1].y

dvx = p[i_1].vx - p[i_2].vx
dvy = p[i_1].vy - p[i_2].vy

ScalarProd = …, MassSum = …, …
```

Mise à jour de la vitesse après la collision

$$\vec{\delta}(t_{coll}) = \vec{r_2}(t_{coll}) - \vec{r_1}(t_{coll})$$

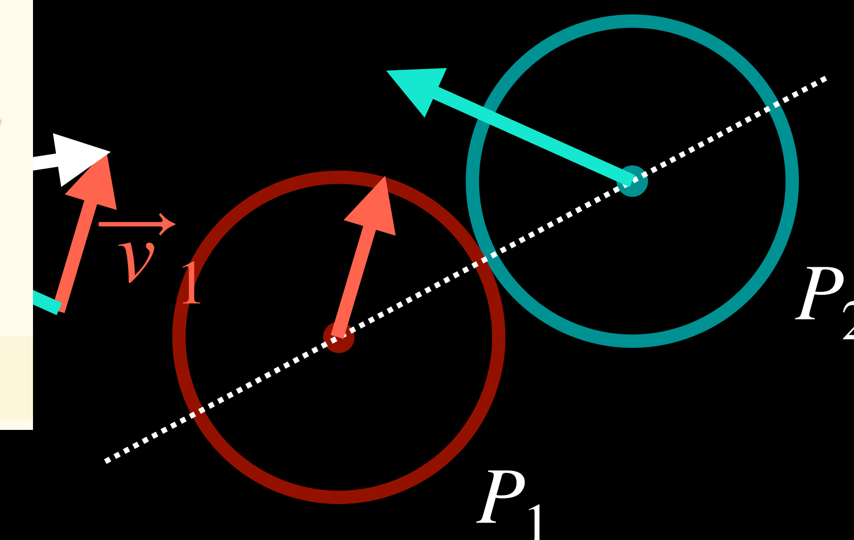


$$\widehat{\vec{\delta}}(t_{coll}) = \frac{\vec{\delta}}{|\vec{\delta}|} \qquad |\vec{\delta}| = \sqrt{\delta_x^2 + \delta_y^2}$$

$$= \cancel{R_1 + R_2}$$

$$\overrightarrow{\Delta v} = \vec{v}_1 - \vec{v}_2$$

```
typedef struct {
    enum col_type type;
    int ia, ib;
    double time;
} Event;
```



$$\boxed{\begin{aligned} \vec{v}\,'_1 &= \vec{v}_1 - \frac{2m_2}{m_1 + m_2}\left(\widehat{\vec{\delta}} \cdot \overrightarrow{\Delta v}\right)\widehat{\vec{\delta}} \\ \vec{v}\,'_2 &= \vec{v}_2 + \frac{2m_1}{m_1 + m_2}\left(\widehat{\vec{\delta}} \cdot \overrightarrow{\Delta v}\right)\widehat{\vec{\delta}} \end{aligned}}$$

https://williamecraver.wixsite.com/elastic-equations

```
dx = p[i_2].x - p[i_1].x
dy = p[i_2].y - p[i_1].y

dvx = p[i_1].vx - p[i_2].vx
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ScalarProd = …, MassSum = …, …
```
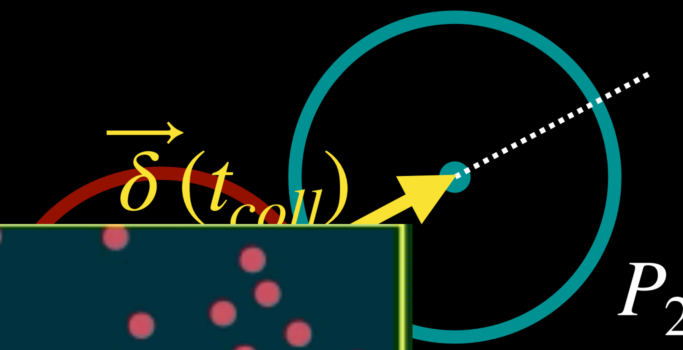
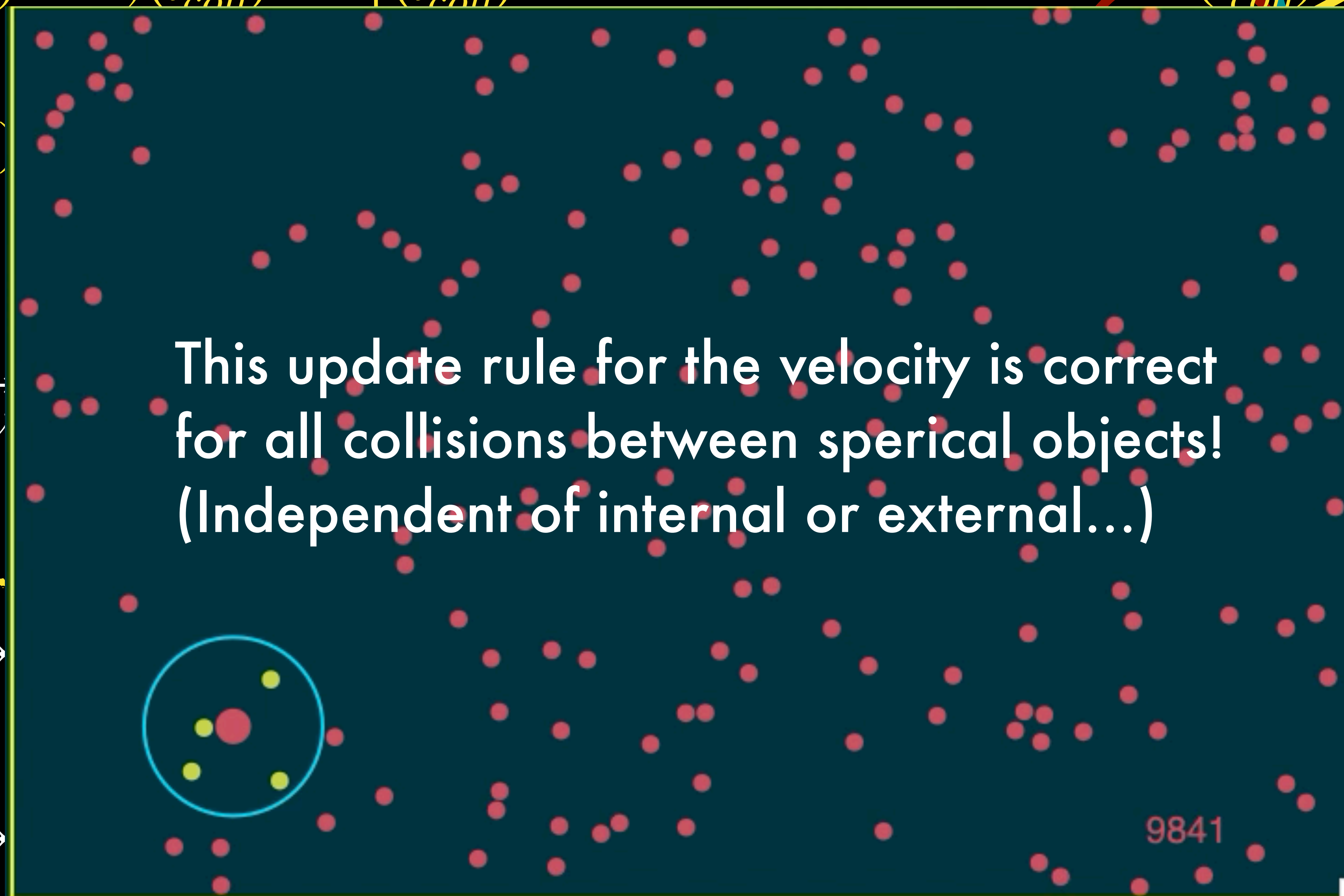
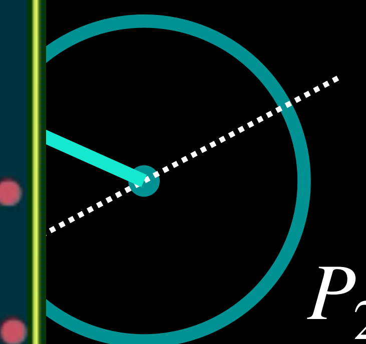

Mise à jour de la vitesse après la collision

$$\overrightarrow{\delta}(t_{coll}) = \overrightarrow{r_2}(t_{coll}) - \overrightarrow{r_1}(t_{coll})$$

$\widehat{\overrightarrow{\delta}}(t_{coll}$







Δv

$\overrightarrow{v}'_1 = \overrightarrow{v}$

$\overrightarrow{v}'_2 = \overrightarrow{v}$

$m_1 + m_2 \Big(\quad \Big)$

```
_1].x
_1].y
i_2].vx
dvy = p[i_1].vy - p[i_2].vy

ScalarProd = …, MassSum = …, …
```

https://williamecraver.wixsite.com/elastic-equations

Comment mesurer ?

Ensemble microcanonique:

$$N = const \quad E = const = \sum_{i=1}^{N} \frac{m_i}{2} \vec{v}_i^{\,2}$$

$$V = const = L_x \times L_y$$

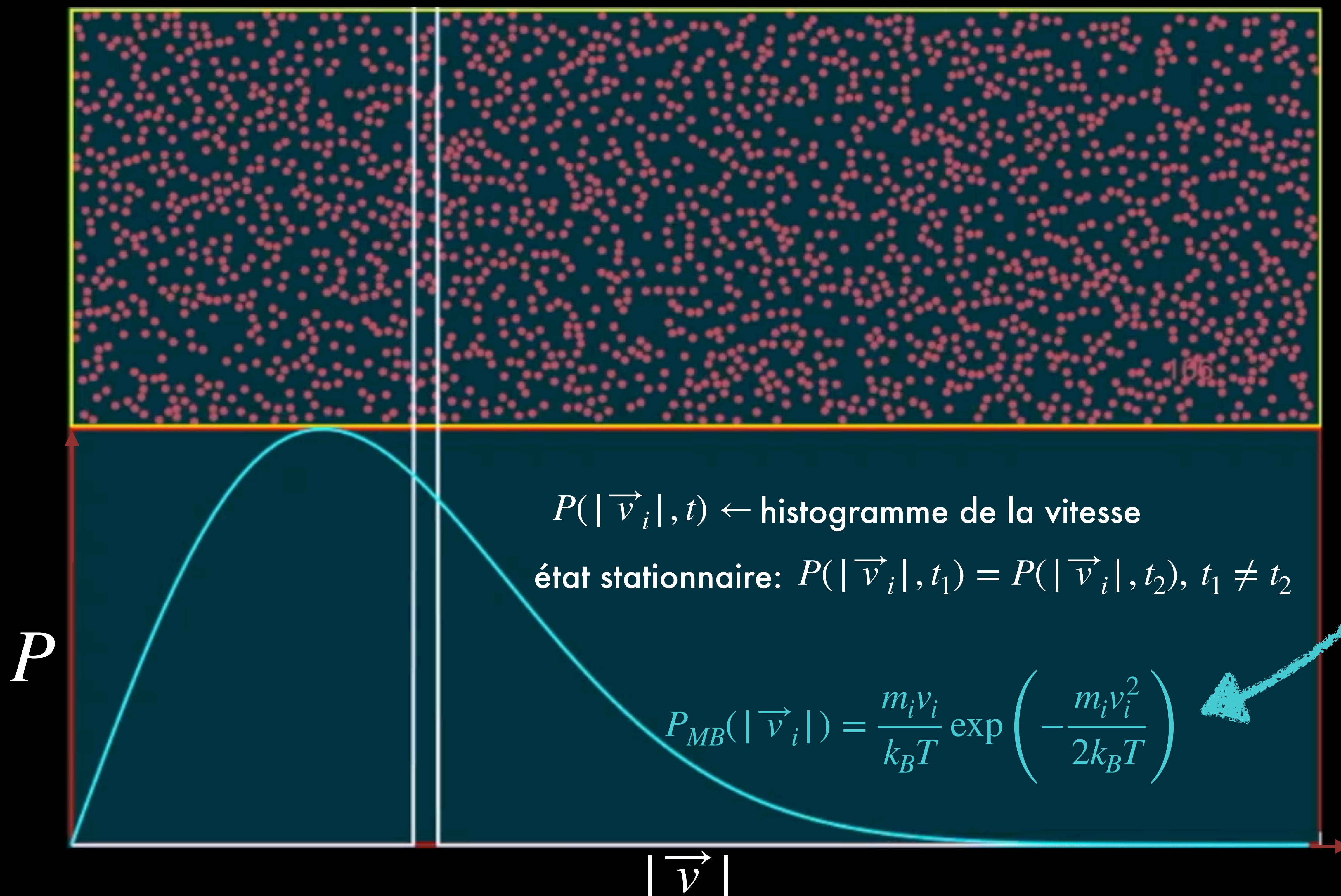
$N \to \infty$

l'équivalence des ensembles

Ensemble canonique:

$$N = const \quad T = const$$

$$V = const = L_x \times L_y$$



Effets de taille finie

$N \to \infty$

l'équivalence des ensembles

Ensemble microcanonique:

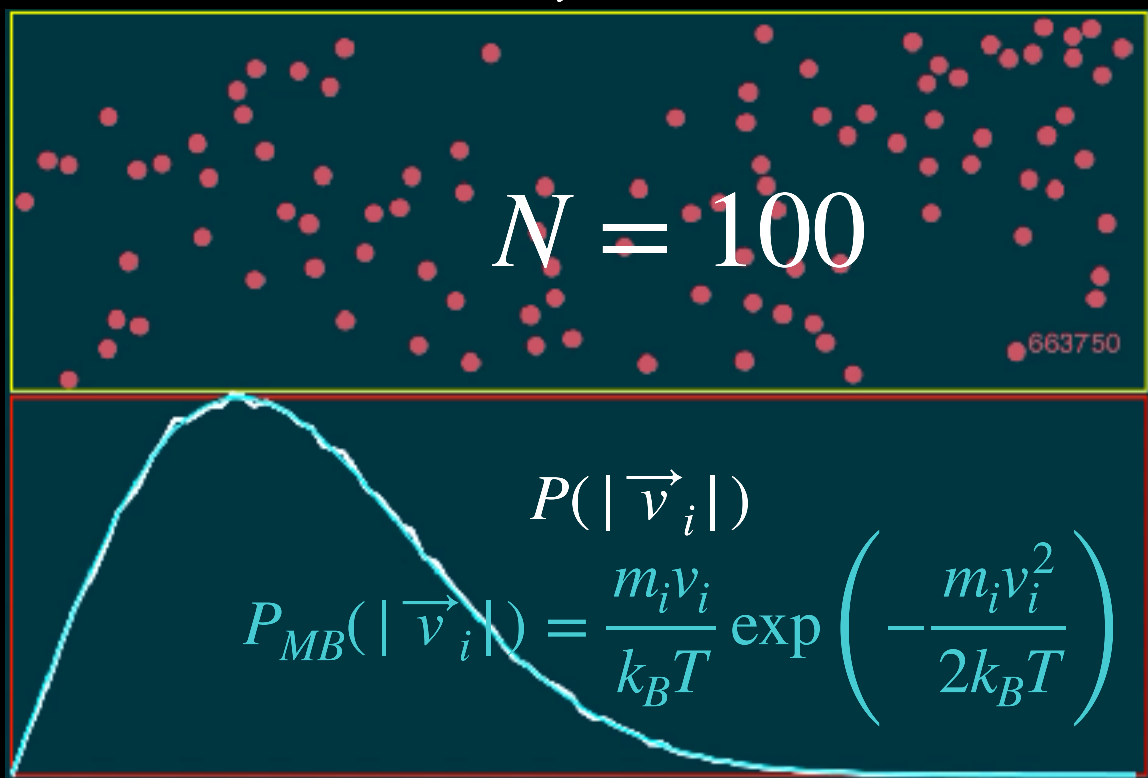
$N = const \quad E = const = \sum_{i=1}^{N} \frac{m_i}{2} \vec{v}_i^{\,2}$

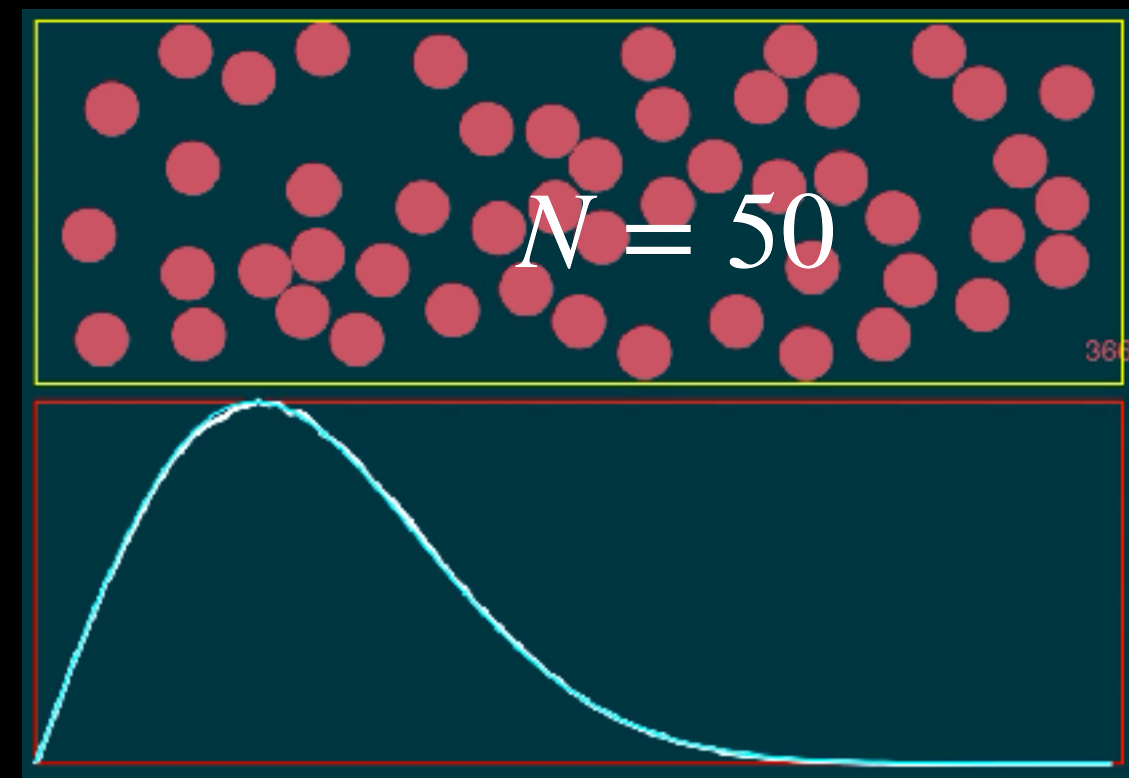
$V = const = L_x \times L_y$

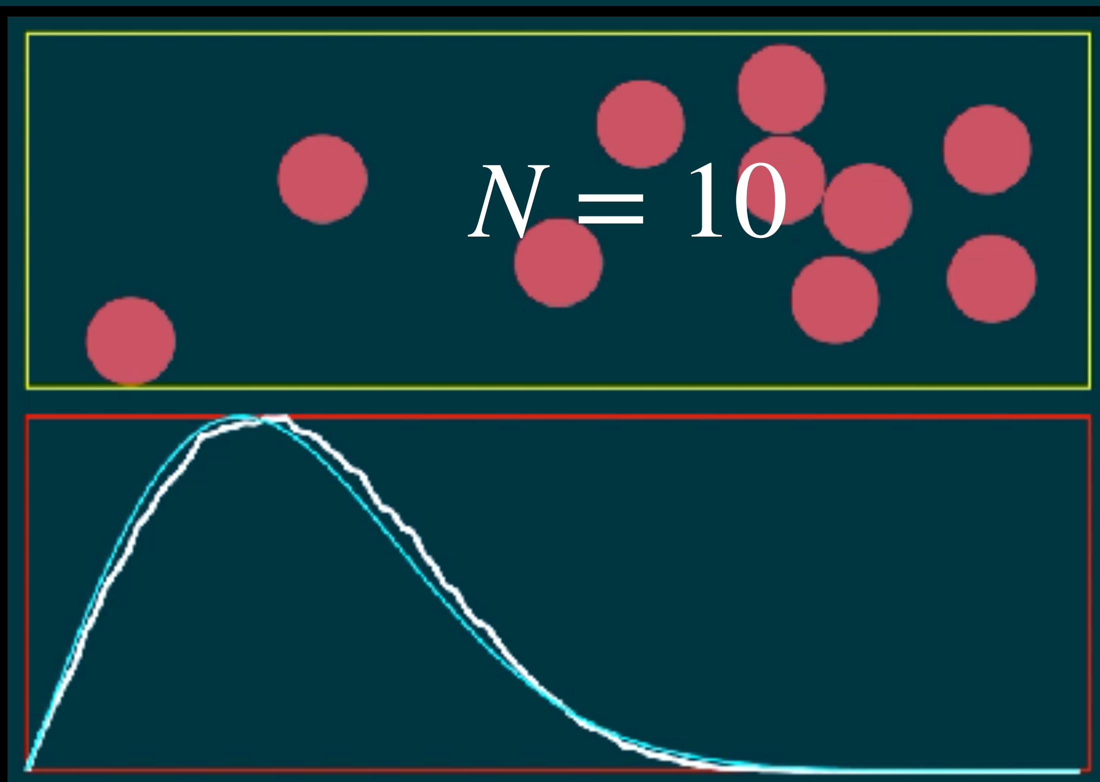
Ensemble canonique:

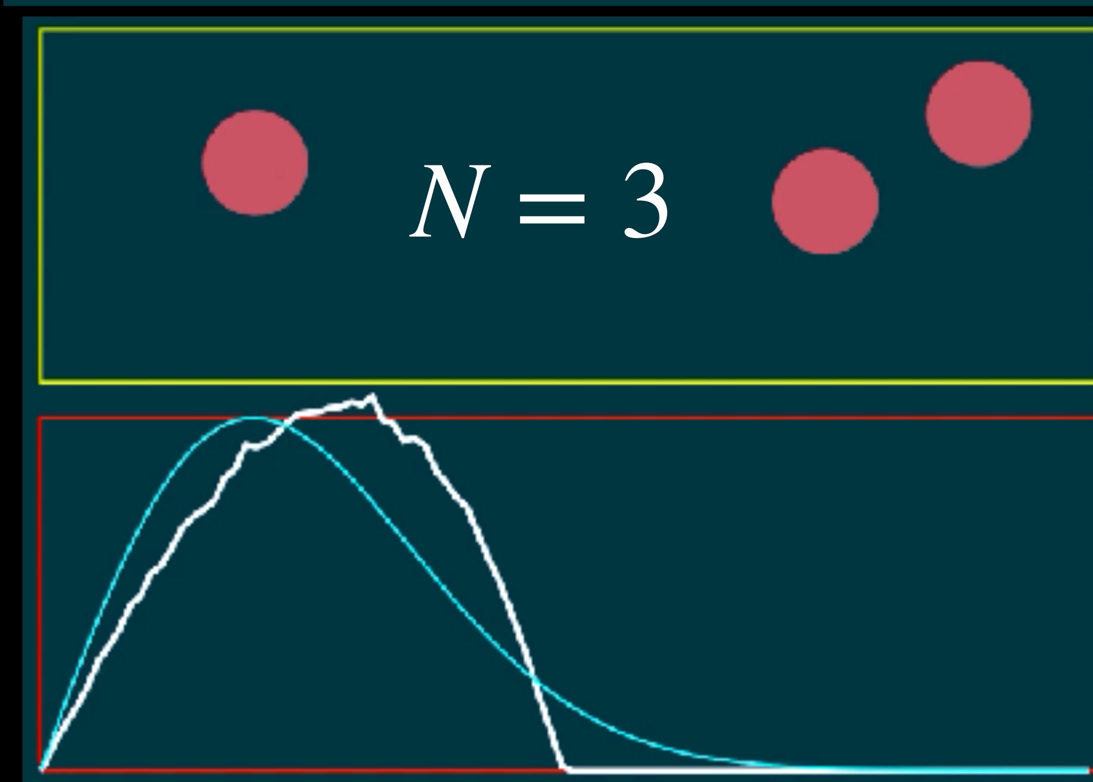
$N = const \quad T = const$

$V = const = L_x \times L_y$









Effets de taille finie

Ensemble microcanonique:

$N = const \quad E = const = \sum_{i=1}^{N} \frac{m_i}{2} \overrightarrow{v}_i^2$

$V = const = L_x \times L_y$

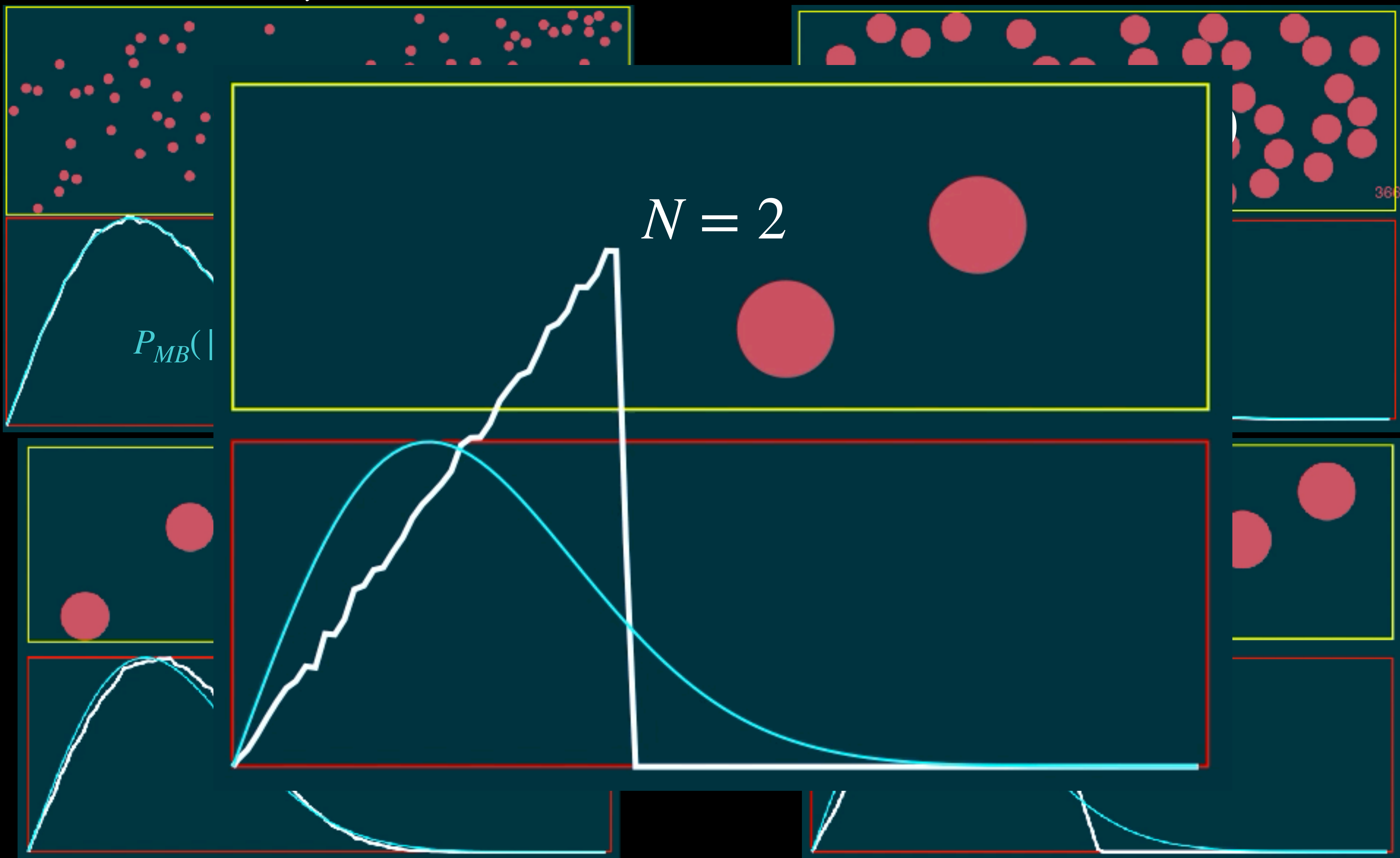
$N \to \infty$

l'équivalence des ensembles

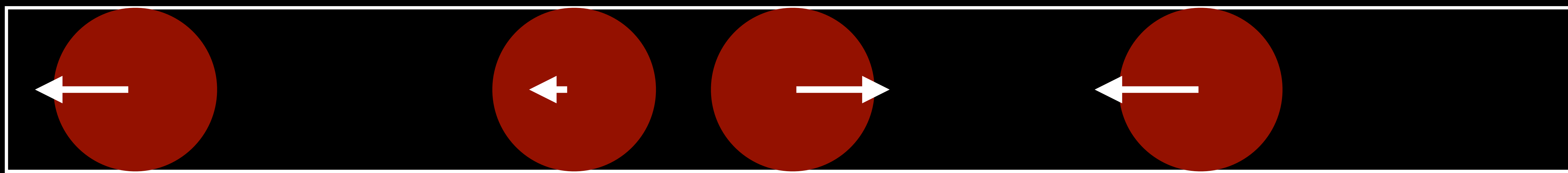
Ensemble canonique:

$N = const \quad T = const$

$V = const = L_x \times L_y$

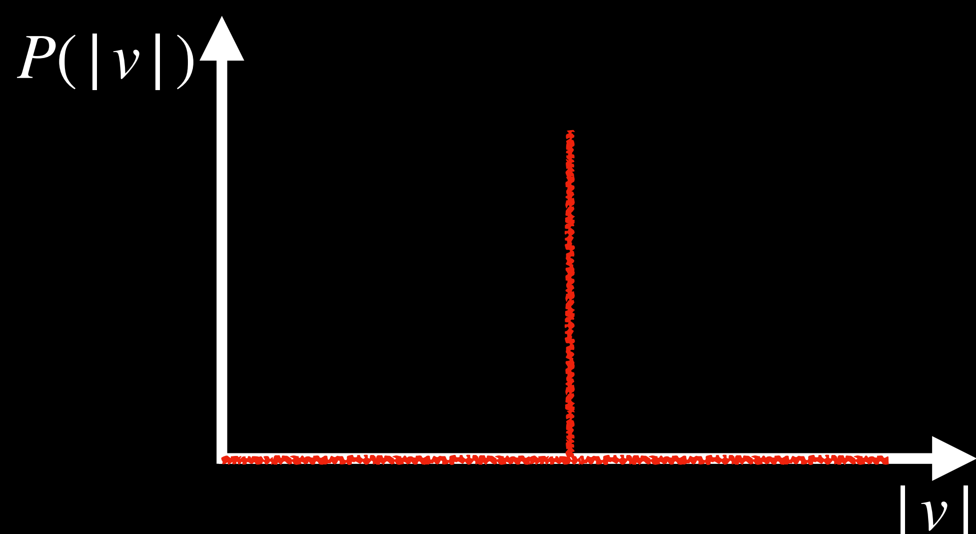


! Question !



Maxwell-Boltzmann 1D: $$P(|v_i|) = 2\sqrt{\frac{m_i}{2\pi k_B T}}\exp\left(-\frac{m_i |v_i|^2}{2k_B T}\right)$$

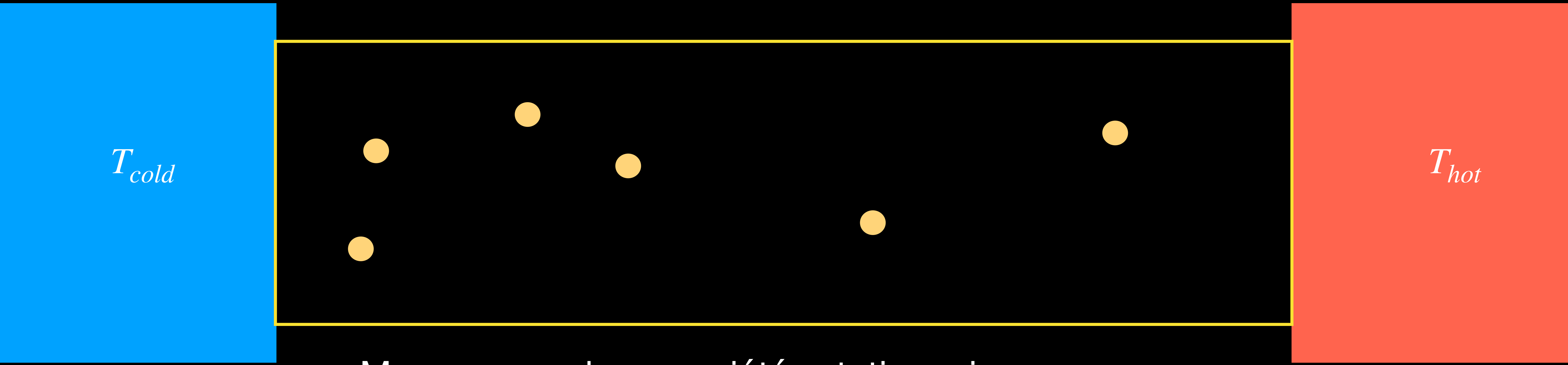
$$m_i = m \longrightarrow \begin{matrix} v'_n = v_m \\ v'_m = v_n \end{matrix} \longrightarrow$$



Une simulation unidimensionnelle de la dynamique moléculaire des disques durs est non-ergodique.

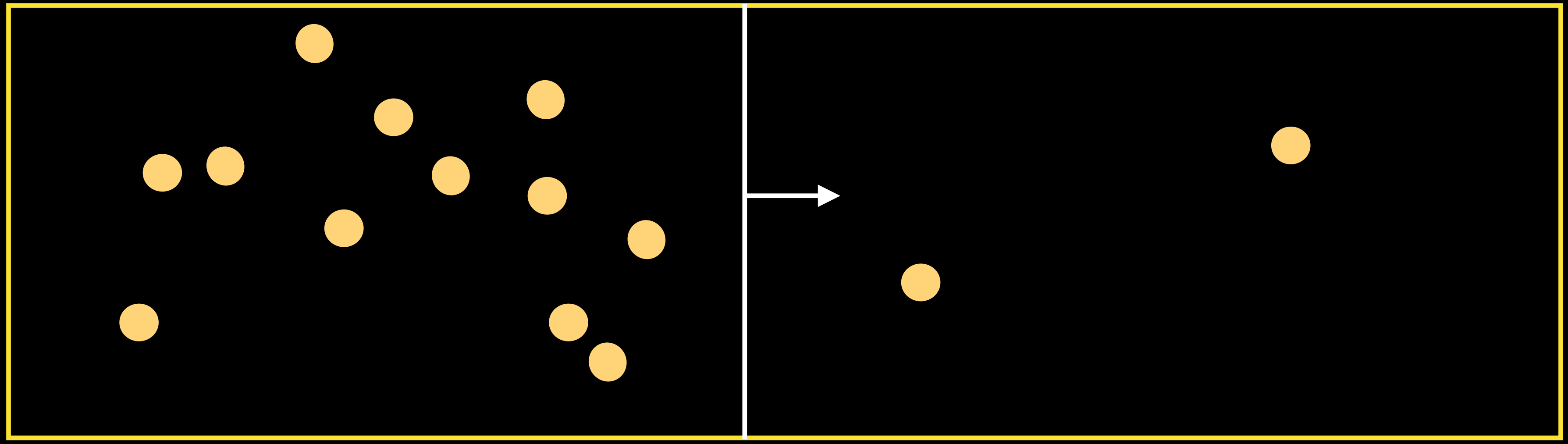
Faire la moyenne correctement.

Etat stationnaire:
par exemple un état stationnaire hors équilibre



Mesures sur des propriétés stationnaires:
Attendez que le système arrive à l'état stationnaire !

Etat non-stationnaire:
(est toujours hors équilibre)



Répétez l'expérience et faites la moyenne sur les différentes réalisations.