The pair of particle may react as follow [3]:

\[ A + B \rightarrow (AB) \rightarrow AB \]

The radiation chemistry code can be used to calculate the reaction rate constants (\( k_{obs}, k_{dif}, k_{act} \)), reaction radii (\( R \)), probability of geminate recombination (\( \alpha \)) for reactions between radiolytic species [5].

In this work, we discuss an approach based on the exact Green functions for diffusion-influenced reactions which may be used to simulate radiation chemistry and eventually extended to study more complex systems, including DNA.

The exact Green functions for an isolated pair are:

\[ \gamma^\pm=\alpha+\beta+\gamma \]
\[ \alpha-\gamma=\alpha-\beta=\beta-\gamma \triangleq \Omega \]
\[ \Omega=\pi/2 \]

The coefficients \( \alpha, \beta, \gamma \) are related to the reaction rate constants (\( k_0=4\pi R D \)):

\[ \alpha=\beta+\gamma=\Omega+2\gamma \]
\[ \alpha=\beta=\gamma=\Omega \]
\[ \alpha=\beta+\gamma=\Omega-\gamma \]
\[ \alpha=\beta=\gamma=\Omega-\beta \]

\[ \alpha=\beta+\gamma=\Omega-\alpha \]
\[ \alpha=\beta=\gamma=\Omega-\alpha \]
\[ \alpha=\beta+\gamma=\Omega-\beta \]
\[ \alpha=\beta=\gamma=\Omega-\beta \]

Many-particles system

- When more particles are added to the system, the number of interactions grow quickly
- 2 Particles
  - 1-2 (1 interaction)
- 3 Particles
  - 1-2, 1-3, 2-3 (3 interactions)
- 4 Particles
  - 1-2, 1-3, 1-4, 2-3, 2-4, 3-4 (6 interactions)
- N Particles
  - N(N-1)/2 interactions \( \Rightarrow \) Grows as \( N^2 \)

The Green Functions can be used to build a radiation chemistry code [4], by using average positions generated by sampling the inter-particle distance at each timestep.

### Chemical reactions and radiolytic yields

- The chemical reactions between radiolytic species with no electrostatic interaction (i.e. their charge product is 0) can be simulated by using the Green Functions described above.
- The radiation chemistry code can be used to simulate the time evolution of the radiolytic species (radiation chemistry) and radiochemical yields [5,6].