Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

1. Linear analysis of Frank's model

The Frank's model presents two steady states (SS), shown in the table SM 1.1 with their respective eigenvalue.

Table SM.1.1 – Steady states and respective eigenvalues

SS	$Eigenvalues$
$(0,0)$	(k_1,k_1)
$(\frac{k_1}{k_2},\frac{k_1}{k_2})$	$(k_1,-k_1)$

As we can see, the steady state (0,0) is characterized by an unstable focus, whereas the steady state $(\frac{k_1}{k_2},\frac{k_1}{k_2})$ is a saddle point. They are represented by the vector field in Figs. SM 1.1 and SM 1.2.

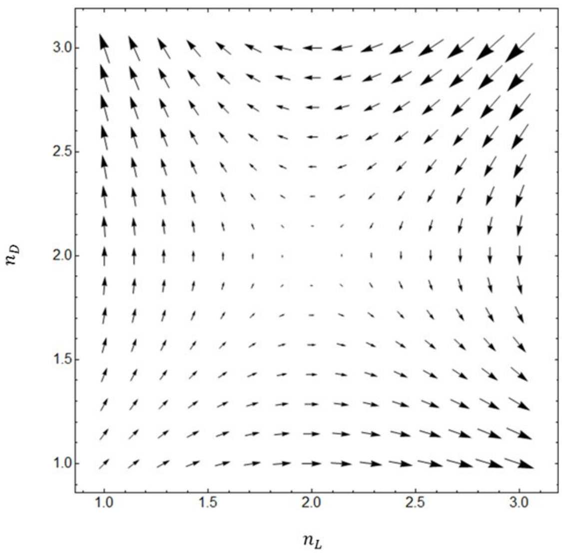

Figure.SM.1.1 – Saddle Point with $k_1 = 1.0$ and $k_2 = 0.5$.

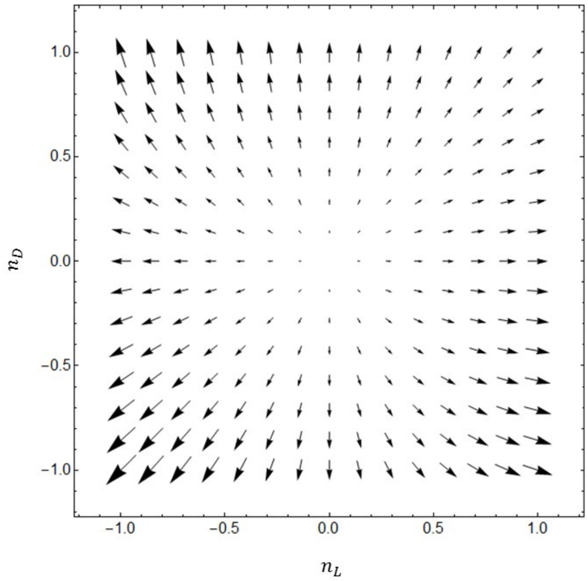

Figure.SM.1.2 – Unstable Focus, with $\kappa_1 = 1.0$ and $\kappa_2 = 0.5$.

2. Probability function

Here, we show the procedure used to obtain the probability equation, Eq. (3).

Initially, we assume the following conditions for the Frank model: $k_1 = k_2 = 0.5,\ N = 100,\ n_D = 1.1$ and $n_L = 1.1 \times \left(1 + \frac{i}{N}\right)$. For each i, where i is one of the integer number $(0,1,2,4,6,8)$, 10^7 trajectories are numerically calculated, and the number of times that each enantiomer composed the final asymmetric state (τ_{n_L} and τ_{n_D}) is computed. The probability of each enantiomer composing the final state is given by the total number of times each enantiomer formed the homoquiral state divided by the total number of trajectories calculated; in other words, $P_L = \tau_{n_L}/10^7$ and $P_D = \tau_{n_D}/10^7$. The probabilities are shown in Table SM.2.1.

Table SM.2.1 – Number of trajectories (10^7) and the probability of each enantiomer composing the final state associated to its enantiomeric excess for $N = 100$

EE	τ_{n_L}	τ_{n_D}	P_L	P_D

.

0*	4963327	4962702	0.4963327	0.4962702
0.011	5610827	4389173	0.5610827	0.4389173
0.022	6173357	3826643	0.6173357	0.3826643
0.044	7205901	2794099	0.7205901	0.2794099
0.066	8075314	1924686	0.8075314	0.1924686
0.088	8747797	1252203	0.8747797	0.1252203

*Probability of racemic final state is $P = (7.40 \pm 0.06) \times 10^{-3}$.

The ratio of probabilities between the specie with initial enantiomeric deficiency by the specie with initial enantiomeric excess ($\frac{P_D}{P_L}$) as a function of the enantiomeric excess is shown in Fig.SM 2.1. These data were interpolatedby an exponential function $\frac{\tau_{n_D}}{\tau_{n_L}} = \frac{P_D}{P_L} = e^{-\alpha EE}$, where $\alpha = 21.78$ was obtained.

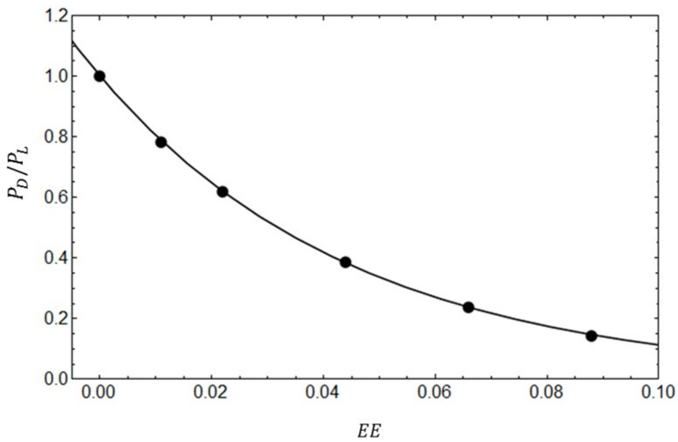

Figure.SM.2.1 –The ratio between probabilities $\frac{P_D}{P_L}$ as a function of the enantiomeric excess is represented by dots and the exponential fitting of the data is represented by the solid line.

The function $P_D = P(EE) = (e^{\alpha EE} + 1)^{-1}$ is represented in Fig. SM2.2.

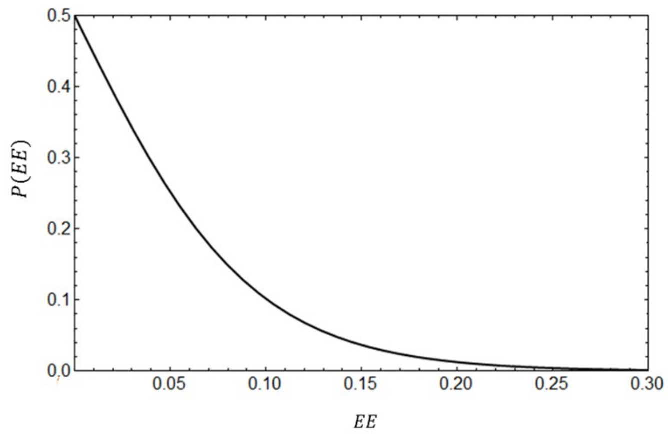

Figure.SM.2.2 – Probability that the enantiomer with initial enantiomeric deficiency will compose the final asymmetric state as a function of the initial EE of the other enantiomer.

3. Dependence of β with k_1 and k_2

Table SM.3.1 – Dependence of β (bold numbers) with k_1 and k_2.

k2 \ k1	0.25	0.375	0.5
0.1	**1.247**	**1.069**	**1.034**
0.125	**1.413**	**1.209**	**1.153**
0.25	**1.947**	**1.621**	**1.585**
0.375	**2.254**	**2.006**	**1.806**

0.5	**2.481**	**2.200**	**2.178**