Supplementary information for ”Ring formation by competition between entropic effect and thermophoresis”

We derive eq. (8) from a lattice model following ref. [11]. We consider random walk of a tracer (colloid) under the presence of other particles (polymers). Both the tracer and the other particles perform random walks on a \( d \)-dimensional regular lattice in which double occupancy of the lattice sites is not allowed. We denote the vector characterizing a jump to the nearest neighbor site \( j \) by \( \vec{b}_j \) (\( j = 1, 2, \ldots, 2d \)) and the jump length by \( b \). The probability at time \( t \) that the site \( \vec{r} \) occupied by a tracer, \( c(\vec{r}, t) \), obeys,

\[
\frac{\partial}{\partial t} c(\vec{r}, t) = \sum_j \left[ \gamma_B \left( \vec{r} + \vec{b}_j \right) P \left( \vec{r} + \vec{b}_j, \vec{r} \phi, t \right) - \gamma_B (\vec{r}) P \left( \vec{r}, \vec{r} + \vec{b}_j \phi, t \right) \right], \quad (a)
\]

where \( \gamma_B (\vec{r}) \) denotes the transition probability and \( P \left( \vec{r} \phi, t \right) \) denotes the joint probability at time \( t \) that the site \( \vec{r} \) is occupied by a tracer and the site \( \vec{r} \) is empty. \( P \left( \vec{r}, \vec{r} \phi, t \right) \) can be rewritten as,

\[
P \left( \vec{r}, \vec{r} \phi, t \right) = c(\vec{r}, t) - P \left( \vec{r}, \vec{r} \phi, t \right), \quad (b)
\]

where \( P \left( \vec{r}, \vec{r} \phi, t \right) \) denotes the joint probability at time \( t \) that the site \( \vec{r} \) is occupied by a tracer and the site \( \vec{r} \) is occupied by another particle. By substituting eq. (b), eq. (a) can be expressed as

\[
\frac{\partial}{\partial t} c(\vec{r}, t) = \sum_j \left[ \gamma_B \left( \vec{r} + \vec{b}_j \right) \left( c \left( \vec{r} + \vec{b}_j, t \right) - P \left( \vec{r} + \vec{b}_j \phi, \vec{r} \phi, t \right) \right) - \gamma_B (\vec{r}) \left( c(\vec{r}, t) - P \left( \vec{r} \phi, \vec{r} + \vec{b}_j \phi, t \right) \right) \right]. \quad (c)
\]

We denote the occupation probability by other particles by \( p(\vec{r}, t) \) and consider the case that the joint probability function can be expressed as,

\[
P \left( \vec{r}, \vec{r} \phi, t \right) = c(\vec{r}, t) p \left( \vec{r}, t \right) \sigma(\vec{r} - \vec{r}), \quad (d)
\]

where the spatial correlation is taken into account by \( \sigma(\vec{r} - \vec{r}) \). By ignoring the spatial variation of \( \sigma(\vec{r}) \) in the limit of small lattice spacing and introducing definition
given by $\sigma(0) = \lim_{b \to 0}(\bar{b}_j)$, we obtain,

$$
\sum_j \gamma_B \left( \bar{r} + \bar{b}_j \right) P \left( \bar{r} + \bar{b}_j \cdot \bar{r}_0, t \right) = \left[ \gamma_B \left( \bar{r} \right) c \left( \bar{r}, t \right) p \left( \bar{r}, t \right) + b^2 p \left( \bar{r}, t \right) \nabla^2 \gamma_B \left( \bar{r} \right) c \left( \bar{r}, t \right) \right] \sigma(0),
$$

(e)

$$
\sum_j P \left( \bar{r} \cdot \bar{r} + \bar{b}_j \cdot \bar{r}_0, t \right) = \left[ c \left( \bar{r}, t \right) p \left( \bar{r}, t \right) + b^2 c \left( \bar{r}, t \right) \nabla^2 p \left( \bar{r}, t \right) \right] \sigma(0).
$$

(f)

When $\gamma_B \left( \bar{r} \right)$ depends on $\bar{r}$ through the spatial variation of temperature, the Soret coefficient can be introduced by

$$
S^c_T = \left( \frac{\partial \gamma_B}{\partial T} \right) / \gamma_B.
$$

(g)

We substitute eqs. (e)-(f) into eq. (c). It is convenient to represent $b^2 p \left( \bar{r}, t \right) \nabla^2 \gamma_B \left( \bar{r} \right) c \left( \bar{r}, t \right)$ in terms of $\nabla \cdot b^2 p \left( \bar{r}, t \right) \nabla \gamma_B \left( \bar{r} \right) c \left( \bar{r}, t \right)$ and $b^2 c \left( \bar{r}, t \right) \nabla^2 p \left( \bar{r}, t \right)$ in terms of $\nabla \cdot b^2 c \left( \bar{r}, t \right) \nabla p \left( \bar{r}, t \right)$.

By further ignoring the spatial dependence in $S^c_T$, eq. (c) in the limit of $b \to 0$ becomes,

$$
\frac{\partial}{\partial t} c \left( \bar{r}, t \right) = \nabla \cdot D^c_B \left[ (1 - \sigma(0)p) \left( cS^c_T \nabla T + \nabla c \right) + \sigma(0)c \nabla p \right],
$$

(h)

where $D^c_B = b^2 \gamma_B$. In the mean field approximation in which $\sigma(0) = 1$, eq. (h) reduces to eq. (8),

$$
\frac{\partial}{\partial t} c \left( \bar{r}, t \right) = \nabla \cdot D^c_B \left[ (1 - p) \left( cS^c_T \nabla T + \nabla c \right) + c \nabla p \right].
$$

(i)

The factor $1 - p$ originates from the vacant probability of a neighboring site in the mean-field approximation. $D^c_B(1 - p)$ represents the tracer diffusion coefficient.

Finally, we would like to add a remark about one component system, where the jump rate of a tracer particle is the same as that of other particles. If we do not distinguish a tracer from other particles, we can set $c \left( \bar{r}, t \right) = p \left( \bar{r}, t \right)$. In this case we obtain,

$$
\frac{\partial}{\partial t} p \left( \bar{r}, t \right) = \nabla \cdot D^c_B \left[ (1 - p)pS^c_T \nabla T + \nabla p \right],
$$

(j)

where $p \left( \bar{r}, t \right)$ is the concentration of Brownian particles including a tracer. In eq. (j) the diffusion coefficient is given by the collective diffusion coefficient $D^c_B$. Equation (j) reduces to that in ref. [1] of the Supplementary information.
References