Two-dimensional diffusion biased by a transverse gravitational force in an asymmetric channel

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Abstract

Using the projection method by Kalinay and Percus [J. Chem. Phys. 122, 204701 (2005)], we derive an effective diffusion coefficient for narrow channels that generalizes previously reported results. This is, a position-dependant diffusion coefficient for two-dimensional asymmetric channels under a transverse gravitational external field is obtained. The main result, shown in equation (5), contains the well-known previous results for symmetric channels with external gravitational force presented by Kalinay [Phys. Rev. E 84, 011118 (2011)], as well as asymmetrical cases where the transverse field goes to zero. Also, found coefficient can be approximately written as an interpolation formula as proposed initially by Reguera and Rubi [Phys. Rev. E 64, 061106 (2001)], can be used to recover preceding results as well. Finally, the excellent agreement of equations (5), (6) and (7) with Brownian dynamics simulations is shown.

Keywords: ICSTCF2021, brownian motion, random walks, confined diffusion

1. Introduction

The diffusion coefficient is a quantity that can be used to describe transport in a system. For a free system, it is customary to use a diffusion constant (D_0). Once confinement or external field influence is imposed, it is needed to extend the model by using the effective diffusive coefficient (D_{eff} or $D(x)$) that, in this case, depends on the x-coordinate. Second Fick's law provides us [1] with a basic description of free systems but Fick-Jacobs [2] and even better, Fick-Jacobs-Zwanzig [3] equations improve the models. Later Reguera and Rubi proposed [4] a new heuristically-found coefficient enhancing Zwanzig's result. Kalinay and Percus used their method [5], named projection method [6] to make an even better description of diffusive systems. The last procedure was used by Kalinay himself [7] to describe a symmetrical channel under transverse gravitational force.

2. Projection Method

A brief outline of the projection method can be stated as follows. We write the bidimentional Smoluchowski equation [8]

$$\frac{\partial \rho(x,y,t)}{\partial t} = \left(D_x \frac{\partial}{\partial x} e^{-\beta U(x,y)} \frac{\partial}{\partial x} e^{\beta U(x,y)} + D_y \frac{\partial}{\partial y} e^{-\beta U(x,y)} \frac{\partial}{\partial y} e^{\beta U(x,y)} \right) \rho(x,y,t), \tag{1}$$

choosing for this particular case a gravitational-like potential $U(y) = Gy$, where $g \equiv \beta G$. Now the one-dimentional density is calculated by taking the integral of the particle density $\rho(x,y,t)$

$$c(x,t) = \int_{h_1(x)}^{h_2(x)} \rho(x,y,t)\, dy. \tag{2}$$

This should be done inside the system's boundaries. The next step is to obtain an equilibrium solution for density by assuming $D_y \to \infty$, this is a transverse-directional equilibrium. This solution can be easily written as

$$\rho_0(x,y,t) = \frac{1}{A(x)}\, e^{-gy} c(x,t), \tag{3}$$

where $A(x)$ is a normalization function that contains boundaries and potential information encoded inside. Now we can see ρ as the result of a perturbative series in $\epsilon \equiv D_x/D_y$

$$\rho(x,y,t) = e^{-gy} \sum_{n=0}^{\infty} \epsilon^n \hat{\omega}_n(x,y,\partial_x) \frac{c(x,t)}{A(x)}, \tag{4}$$

applying the usual techniques for series solutions and the key assumption of a stationary regime for long times ($\partial_t c(x,t)$) we can found $D(x)$.

3. Results

The known results for two-dimensional narrow channels could be generalized by

$$\begin{aligned} \frac{D(x)}{D_0} = 1 &- \frac{w'^2(x)}{4\sinh^2\left[\frac{1}{2} g w(x)\right]} \\ &\times \left\{ 1 + \cosh^2\left[\frac{1}{2} g w(x)\right] - g w(x) \coth\left[\frac{1}{2} g w(x)\right] \right\} \\ &- y_0'(x) \left\{ y_0'(x) - w'(x) \coth\left[\frac{1}{2} g w(x)\right] \right. \\ &\left. + \frac{1}{2} g w(x) w'(x) \operatorname{csch}^2\left[\frac{1}{2} g w(x)\right] \right\}, \end{aligned} \tag{5}$$

and approximately written using an interpolation formula

$$D_\eta(x) = \frac{D_0}{\left[1+\frac{1}{4}w'^2(x)\right]^\eta}, \tag{6}$$

where

$$\eta = \frac{1}{\sinh^2\left[\frac{1}{2}gw\right]}\left\{1+\cosh^2\left[\frac{1}{2}gw\right] - gw\coth\left[\frac{1}{2}gw\right]\right\} + 4\frac{y_0'}{w'^2}\left\{y_0' - w'\coth\left[\frac{1}{2}gw\right] + \frac{1}{2}gww'\operatorname{csch}^2\left[\frac{1}{2}gw\right]\right\}. \tag{7}$$

Above equations contains the channel width $w(x) = h_2(x) - h_1(x)$, the midline $y_0(x) = [h1(x)+h_2(x)]/2$ and their respective derivatives.

4. Brownian Dynamics Simulations

Simulations where performed using Fortran & C codes, parallelizing the exection of the programs. All realizations were made with $\Delta t = 10^{-6}$, 10^7 steps and 2.5×10^4 particles. The probe channels has a period of $L = 1$. First simulation round was conducted with channel boundaries' defined by $h_2(x) = [\sin(2\pi x)+1.02]/(2\pi) = -h_1(x)$ and a G magnitude transversal force. Following simulations were completed changing the lower boundary to be $h_1(x) = 0$ and transversal constant force in two different directions $+G$ and $-G$.

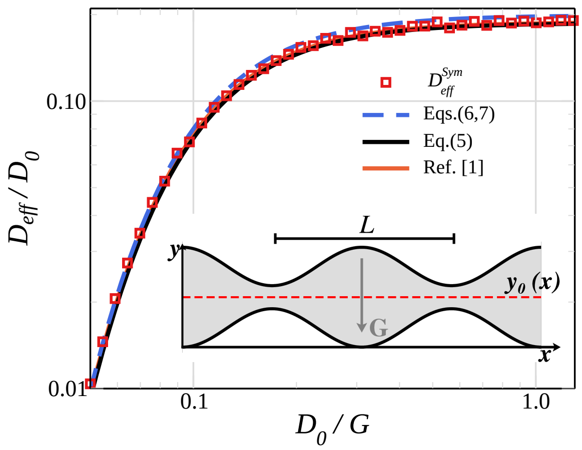

Figure 1: Effective diffusion coefficients obtained numerically in Ref. [9] (continuous red line), those predicted by equation (5) (continuous black line), and the interpolation formula given by equations (6) and (7) (dashed blue line), are compared with the values obtained by Brownian dynamics simulations (square red symbols). The boundaries of the channel are defined by the dimensionless function $h_2(x) = -h_1(x) = [\sin(2\pi x)+1.02]/2\pi$, subjected to a constant perpendicular G force. L gives the periodicity of the channel [9]. In the inset the straight midline is shown as a red dotted line.

5. Conclusions

The newly obtained Eq. (5) allows us to recover the Kalinay results [7] by considering a symmetric channel with zero midline. Reguera and Rubi expression [4] arises when the transversal force is null. Also, Bradley model [10] can be gathered if the asymmetry of the system is maintained but the transverse external field is removed. Some interesting behavior is predicted for the diffusion coefficient by setting $G\to-\infty,+\infty$, where $D_0/\left[1+h_2'^2(x)\right]$ and $D_0/\left[1+h_1'^2(x)\right]$ respectively, this can be promising in order to achieve particle separation and diffusion coefficient control at will by turning on and off the external field or tuning its magnitude.

Also, it is remarkable how Eq. (5) can be recovered by taking the first two terms of the series obtained from Eqs. (6) and (7) as Reguera and Rubi [4], and Kalinay [7] proposed. Furthermore, the asymmetry and boundaries information of the system can be encoded into the η exponent.

The Brownian dynamics simulations and Eqns. (5), (6), and (7) are in excellent agreement. Additionally, the symmetrical case was compared to the predicted behavior found by another methods as shown in Ref. [9].

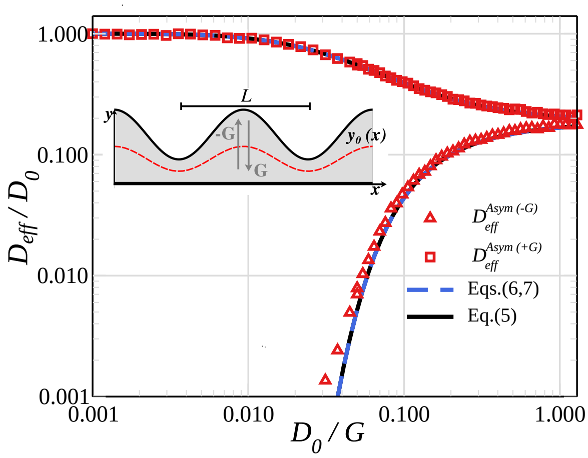

Figure 2: Effective diffusion coefficients predicted by equation (5) (continuous black line), and the interpolation formula given by equations (6) and (7) (dashed blue line), are compared with the values obtained by Brownian dynamics simulations (red square and triangle symbols). The boundaries of the channel are defined by the dimensionless function $h_2(x) = [\sin(2\pi x)+1.02]/2\pi$ and $h_1(x) = 0$, subjected to a constant perpendicular G force. L gives the periodicity of the channel [9]. In the inset the curved midline is shown as a red dotted line.

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