

On the geometrical description of the effective diffusion in confined environments: 3D channels

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Diffusion of Brownian particles in bounded channels is a fundamental problem in physics. A particular case is a 2D channel formed by two smooth functions as its boundaries. In this case, due to a perturbative expansion and the definition of the effective diffusion, we can managed to obtain an expression of the effective diffusion coefficient [1], in the sense of Zwanzig [2].

In this contribution we present the generalization of our previous results [1] for the 3D case. To this end we employ the formalism of Frenet-Serret vectors which can be used to construct 3D channels. In this construction, we can naturally define a coordinate transformation in which an arbitrary smooth channel is mapped into a cylinder-like tube. Thus, the Fick equation gets modified when is written in this coordinates. Then, by employing the boundary conditions, we identify a position dependent diffusion coefficient. In this case, we consider reflecting boundaries conditions as usual in this systems [3].

Finally we calculate the diffusion coefficient for some specific examples. We compare our analytic solutions with previous expression in the literature [3] as well as numerical Brownian simulations, obtaining a remarkable agreement.

References

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