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VALIDATING THE DIFFUSION APPROXIMATION THROUGH CONDITIONAL ENTROPIES

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The diffusion approximation replaces a real transport dynamics by an approximate stochastic Markov process. It is proposed that, when both dynamics have invariant measures, the conditional entropy of the invariant measure of the real dynamics with respect to the invariant measure of the Markov process be used to assess quantitatively the validity of the approximation. This proposal is tested on particle transport; the diffusion approximation is found to be quite robust, valid for an unexpectedly large range of mass ratios between the solvent and the Brownian particle.

 $\mathit{Keywords}:$ Kinetic and transport theory of gases; Stochastic analysis methods; Brownian motion.

1. Introduction

Markov processes are ubiquitous in scientific modeling, with applications ranging from physics and chemistry¹ to economics,² through biology^{3–6} and population dynamics.⁷ In physics, Markov processes can be used as an approximate description of diffusive transport, valid when the mass of the transported object is much larger than the mass of the solvant particles.⁸ Though very well-known, this qualitative statement still lacks a quantitative counterpart. Indeed, such a counterpart would presuppose the existence of a method to assess quantitatively the validity of the diffusion approximation, and no such method has been proposed yet.

The aim of this letter is twofold: (i) to propose a new, quantitative method to assess theoretically the validity of the diffusion approximation, (ii) to use this method to determine how the mass ratio r between the transported particle and the solvent particles influences the validity of the approximation.

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Here is a brief summary of how these two goals are implemented and of the conclusions that are reached. According to kinetic theory,^{8,10} diffusion is induced by collisions between the solvent particles and the transported ones. In the diffusion approximation,⁸ the net, global effect of these collisions on a transported particle is modeled by a Markov stochastic process¹¹ which is fully determined by the underlying kinetic model. This process generally admits a certain equilibrium distribution Φ_E in velocity space, while the more precise, kinetic description (typically, the Boltzmann equation) admits the usual Maxwell–Boltzmann distribution Φ_M as equilibrium law.¹⁰ The difference of information content between Φ_M and Φ_E can be measured theoretically^{12,13} by the conditional entropy S_c of Φ_M with respect to Φ_E . We propose to assess the validity of the diffusion approximation by the numerical value of this conditional entropy. Goal (ii) is then implemented by explicitly computing the conditional entropy S_c as a function of the mass ratio r between the transported particle and the solvent particles. This reveals that the diffusion approximation is actually quite robust. For example, with a mass ratio $r = 10^{-2}$ (transported particles are only 100 times heavier than solvant particles), the conditional entropy S_c is as low as 2.2×10^{-4} .

2. The Diffusion Approximation

Consider a solvent S made of particles of mass m_S , conveniently called S-particles, in which particles of mass m_B , conveniently called Brownian or B-particles, are transported by short-range interactions with the S-particles. We suppose that there are sufficiently few B-particles in S to neglect interactions between B-particles and between more than one B- and one S-particle at a time. All the properties of transport can then be recovered by studying the motion of a single, arbitrary B-particle and the statistical properties of this motion are entirely characterized by the solvent one-particle distribution and the law fixing the short-range interaction between a B and an S-particle. We neglect the internal structure of B-particles and assume that the short-range interaction between a B- and an S-particle can be modeled as an elastic collision between hard spheres and that the associated sphere radii are R_S and R_B . We also assume, in accordance with standard kinetic theory, that the solvent one-particle distribution is Maxwellian.

In the above model, the trajectory of a *B*-particle is a succession of line segments started and ended by collisions with *S*-particles. At a fixed initial momentum \mathbf{p} of the *B*-particle before such a collision, the momentum loss \mathbf{q} of the *B*-particle during the collision is a random variable whose distribution depends on the collision cross-section and on the distribution of *S*-particles. Diffusions are by definition governed by Langevin-like equations (Ito processes¹¹) and these are driven by Gaussian noises. Approximating the motion of a *B*-particle by a diffusion thus comes down to approximating, for each \mathbf{p} , the distribution of the momentum loss \mathbf{q}_B by a Gaussian. The law of a stochastic process defined by such a Langevin equation is described by a distribution function Φ of the time t and of the position **r** and velocity **v** of a *B*-particle; this function obeys the Fokker–Planck equation^{1,11}:

$$\frac{\partial \Phi}{\partial t} + v^i \frac{\partial \Phi}{\partial r^i} = \frac{1}{m_B} \frac{\partial}{\partial v^i} \left(-F^i \Phi + \frac{1}{m_B} \frac{\partial}{\partial v^j} (D^{ij} \Phi) \right),\tag{1}$$

where **F** is the deterministic part of the force experienced by the *B*-particle, and D is the noise tensor. This force **F** and the noise tensor D can be computed from the expectation (mean value) of **q** and **q** \otimes **q** respectively.⁹ This delivers:

$$\mathbf{F} = -\alpha_0(v)\mathbf{v}, \quad \text{and} \quad D = \sigma_0(v)\mathcal{E} + \sigma_2(v)\mathbf{v} \otimes \mathbf{v}$$
(2)

where \mathcal{E} is the (inverse) Euclidean metric tensor ($\mathcal{E}^{ij} = 1$ if i = j and 0 otherwise). Naturally, all coefficients introduced above also depend on the masses m_B and m_S , and on the characteristic radii R_B and R_S . The expressions of the coefficients in (2) are more readable if the following conventions are done:

- **u** denotes the dimensionless velocity of the *B*-particles: $\mathbf{u} = \mathbf{v}\sqrt{m_S/k_BT}$. Note that the velocity scale k_BT/m_S chosen to make **u** dimensionless is the thermal velocity of *S*-particles. Thus, when the *B*-particles have a much larger mass than the *S*-particles, $|\mathbf{u}|$ is much smaller than unity.
- u and v denote the moduli of \mathbf{u} and \mathbf{v} .
- μ denotes $(m_S^{-1} + m_B^{-1})^{-1}$.
- $\xi(x)$ stands for $e^{-\frac{x^2}{2}}$, and $\zeta(x)$ for $\sqrt{\frac{\pi}{2}} \frac{\operatorname{erf}(x/\sqrt{2})}{x}$, where analytical continuation is implied for x = 0.

With this notation, the exact expressions for the coefficients in (2) are:

• Friction coefficient:

$$\alpha_{0}(v) \equiv \tilde{\alpha}_{0}(u) = n_{S} \sqrt{\frac{2\pi k_{B}T}{m_{S}}} \mu (R_{B} + R_{S})^{2} \\ \times \left(\frac{-1 + 2u^{2} + u^{4}}{u^{2}} \zeta(u) + \frac{1 + u^{2}}{u^{2}} \xi(u)\right).$$
(3)

• Noise coefficient:

$$\sigma_0(v) \equiv \tilde{\sigma}_0(u) = \frac{1}{12\pi} n_S \left(\frac{2\pi k_B T}{m_S}\right)^{\frac{3}{2}} \mu^2 (R_B + R_S)^2 \\ \times \left(\frac{-3 + 9u^2 + 9u^4 + u^6}{u^2} \zeta(u) + \frac{3 + 8u^2 + u^4}{u^2} \xi(u)\right).$$
(4)

• Second-order noise coefficient:

$$\sigma_2(v) \equiv \tilde{\sigma}_2(u) = \frac{1}{2} n_S \sqrt{\frac{2\pi k_B T}{m_S}} \mu^2 (R_B + R_S)^2 \\ \times \left(\frac{3 - 3u^2 + 3u^4 + u^6}{u^4} \zeta(u) + \frac{-3 + 2u^2 + u^4}{u^4} \xi(u)\right).$$
(5)



Fig. 1. Invariant measure of the diffusion process for a mass ratio r = 0.01, as a function of the dimensionless velocity v/v_0 with $v_0 = \sqrt{k_B T/m_B}$ (solid curve). The corresponding Maxwellian distribution is plotted on the dashed line. The scale of the vertical axis is arbitrary.

3. Invariant Measure of the Diffusion Process

The density Φ_E of the invariant measure with respect to the Lebesgue measure d^3v obeys:

$$\frac{\partial}{\partial v^i} \left(-F^i \Phi_E + \frac{1}{m_B} \frac{\partial}{\partial v^j} (D^{ij} \Phi_E) \right) = 0.$$
(6)

By isotropy, the solution of (6) can be expressed as a function of the modulus v of the velocity: $\Phi_E(\mathbf{v}) = \phi(v)$. Inserting this form into the above equation leads to:

$$A(v)\phi(v) + B(v)\phi'(v) = 0,$$
(7)

where $\phi'(v)$ stands for the derivative of ϕ with respect to v. In (7), the coefficients A(v) and B(v) are:

$$A(v) = \alpha_0(v) + \frac{1}{m_B} \left(\frac{\sigma'_0(v)}{v} + v\sigma'_2(v) + 4\sigma_2(v) \right),$$
(8)

and

$$B(v) = \frac{1}{m_B} \left(\frac{\sigma_0(v)}{v} + v \sigma_2(v) \right).$$
(9)

The solution of (7) is

$$\phi(v) = \phi_0 \exp\left[-\int_0^v \frac{A(\nu)}{B(\nu)} d\nu\right],\tag{10}$$

the constant ϕ_0 being determined by the normalization condition $\int_0^\infty \phi(v) 4\pi v^2 dv =$ 1. The function $\phi(v)$ can be determined numerically for all values of the mass ratio r; it is plotted in Fig. 1 for r = 0.01 (Brownian particles are 100 times heavier than solvent particles), together with the corresponding Maxwellian distribution.

4. Conditional Entropy

The real, physically relevant equilibrium distribution of a *B*-particle in velocity space is not Φ_E but the standard Maxwell-Boltzmann distribution:

$$\Phi_M(\mathbf{v}) = \left(\frac{2\pi k_B T}{m_B}\right)^{-\frac{3}{2}} \exp\left(-\frac{m_B v^2}{2k_B T}\right).$$
(11)

The conditional or Kullback entropy $S_c [\Phi_M / \Phi_E]$ of Φ_M with respect to Φ_E is defined by the following relation^{12,13}:

$$S_c \left[\frac{\Phi_M}{\Phi_E} \right] \equiv \int_{\mathbb{R}^3} \Phi_M(\mathbf{v}) \ln \left(\frac{\Phi_M(\mathbf{v})}{\Phi_E(\mathbf{v})} \right) d^3 v \,. \tag{12}$$

Roughly speaking, this entropy measures the difference of information content between Φ_M and Φ_E and it can serve as a quantitative estimate of the error made in approximating the real transport by a diffusion process. Indeed, if both distributions are close to each other, say symbolically $\Phi_E(\mathbf{v}) = \Phi_M(\mathbf{v})(1 + \epsilon(\mathbf{v}))$ with $\epsilon \ll 1$, then

$$S_c \left[\frac{\Phi_M}{\Phi_E} \right] \simeq \int_{\mathbb{R}^3} \Phi_M(\mathbf{v}) (\epsilon(\mathbf{v}))^2 d^3 v \,, \tag{13}$$

and the conditional entropy then measures the mean value or average of the squared discrepancy between the Φ_E and Φ_M . Thus, the smaller the conditional entropy, the better the diffusion approximation. Note that the definition of $S_c[\Phi_M/\Phi_E]$ is asymmetrical between Φ_E and Φ_M and that $S_c[\Phi_M/\Phi_E]$ makes more physical sense than $S_c[\Phi_M/\Phi_E]$ because it makes more sense to compute the above average by using the true equilibrium measure $\Phi_M d^3 v$ rather than the approximation $\Phi_E d^3 v$.

The conditional entropy $S_c[\Phi_M/\Phi_E]$ is plotted in Fig. 2 against the mass ratio r. This plot shows that the diffusion approximation is actually quite robust. For



Fig. 2. Conditional entropy $S_c[\Phi_M/\Phi_E]$ of Φ_M with respect to Φ_E , as a function of the mass ratio $r = m_S/m_B$.

example, with a mass ratio as high as r = 0.01 (Brownian particles are only 100 times heavier than solvent particles), the conditional entropy $S_c[\Phi_M/\Phi_E]$ is as low as 2.2×10^{-4} . But Fig. 2 also displays the breakdown of the diffusion approximation. Indeed, a mass ratio of r = 1 leads to a conditional entropy of order 0.3, which means that, for this mass ratio, Φ_M/Φ_E is of order 1.3 when v stays inside the central peak of the Gaussian Φ_M ; the corresponding mean relative difference between Φ_M and Φ_E is thus around 30%.

It is interesting to notice that neither Φ_M nor Φ_E depend on the radii of the Brownian and solvant particles. This is seen explicitly from (11) for Φ_M . As for Φ_E , the coefficients α_0 , σ_0 and σ_2 entering the definition of A and B all depend linearly on the square $(R_B + R_S)^2$ and this dependence thus cancels form the quotient A/Band, therefore, from Φ_E too. Consequently, the conditional entropy $S_c [\Phi_M/\Phi_E]$ does not depend on the radii of the Brownian and solvant particles.

5. Conclusion

The diffusion approximation comes down to modeling diffusive transport by a Markov stochastic process. In dilute gas, the real equilibrium Maxwell–Boltzmann distribution Φ_M is then replaced by another distribution, say Φ_E . We have suggested that the validity of the diffusion approximation can be measured quantitatively by the conditional entropy of Φ_M with respect to Φ_E . This entropy has been computed as a function of the mass ratio between the transported particle and the solvent particles. The conclusion is that the diffusion approximation is actually quite robust; for example, a mass ratio of 0.01 corresponds to a conditional entropy of 2.2×10^{-4} .

Let us conclude by listing a few natural extensions to this work. One should first investigate if the validity of the diffusion approximation can be quantitatively assessed by other measures than equilibrium conditional entropies and, if that is the case, how these measures compare with each other. The computation presented in this letter should also be extended to deal with situations where the basic kinetic model is more general than the Boltzmann one. Finally, assessing the validity of the diffusion approximation is also important in the relativistic regime, to deal for example with runaway electrons^{18,19} and transport in both astrophysical and non-astrophysical plasmas.^{20,21}

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