

Reliability of fluctuation-induced transport in a Maxwell-demon-type engine

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Abstract

We study the transport properties of an overdamped Brownian particle which is simultaneously in contact with two thermal baths. The first bath is modeled by an additive thermal noise at temperature T_A . The second bath is associated with a multiplicative thermal noise at temperature T_B . The analytical expressions for the particle velocity and diffusion constant are derived for this system, and the reliability or coherence of transport is analyzed by means of their ratio in terms of a dimensionless Péclet number. We find that the transport is not very coherent, though one can get significantly higher currents.

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I. INTRODUCTION

The second law of thermodynamics implies that it is not possible to get useful work from a single heat bath at constant temperature. The perfect time-reversal symmetry (or detailed balance) which exists under equilibrium conditions causes the flux in either direction to be the same resulting in zero average flux. But advances in this area, especially in the context of biological systems, show that it is possible to induce a directed motion provided there exist some nonequilibrium fluctuations. These are usually provided by unbiased external input agents. Devices which exploit these fluctuations to generate a unidirectional flow have been termed as ratchets or Brownian motors. For a detailed discussion of these systems, see [1].

The underlying thermal fluctuations are usually quantified in terms of temperature. Though these fluctuations cannot be observed directly in macroscopic systems, the recent advances in nanotechnology and molecular biology allow one to devise molecular systems where they play a pivotal role. Thus, rather than trying to avoid these inherent fluctuations, they have been utilized for constructive purposes: Brownian motors serve as the best example of this.

Many different classes of model systems exist in the literature, and detailed studies have been done with regard to transport and energetics in such systems. In our present work, we consider a model of Brownian motor where the system has a space-dependent diffusion coefficient $D(x)$. The main emphasis in these systems is that the potential need not be ratchet-like. Examples of such systems arise in semiconductor and superlattice structures, molecular motor proteins moving along microtubules, etc. [2, 3].

A space-dependent diffusion coefficient $D(x)$ could arise either due to a spatial variation of temperature or friction coefficient, or both. For a system having a space-dependent temperature $[T(x)]$ the system dissipates energy during its evolution differently at different places. This implies that the system is out of equilibrium. A similar effect arises in a medium with a space-dependent friction coefficient $[\eta(x)]$ in the presence of an external noise [4–8]. To be more precise, frictional inhomogeneity does not generate any current by itself - nonequilibrium fluctuations are crucial for transport in these systems.

It has been shown by Büttiker [8] that, in the presence of $D(x)$, the Boltzmann factor

$\exp[-V(x)/k_B T]$ has to be generalized as $\exp[-\psi(x)]$ where

$$\psi(x) = - \int^x dq \frac{v(q)}{D(q)}. \quad (1)$$

Here, $v(x) = -\mu dV/dx$ is the drift velocity and μ is the mobility. For a homogeneous system, $D(x)$ is given by Einstein's relation $D = \mu k_B T$. The stability and dynamics of nonequilibrium system is greatly influenced by the above generalized potential. Here, one has to invoke the notion of global stability of states, as opposed to local stability which is valid for equilibrium states [7].

In the present work, we consider a Brownian particle in contact with two thermal baths, A and B . The underlying potential $V(x)$ and the friction coefficient $\eta(x)$ are periodic in space, and separated by a phase difference other than 0 and π . We study the quality of transport in such systems. Here, the unidirectional current arises due to a combination of both $\eta(x)$ and the fluctuations present in the second thermal bath.

Millonas [5] and Jayannavar [6] have analyzed the basic framework for particle transport in such systems. Subsequently, Chaudhuri et al. [9] have also studied this model with modifications in the bath parameters. However, there has been no systematic analysis of the dependence of the current on system parameters. Further, there is no clear understanding of the coherence of transport in these systems. In this paper, we undertake a detailed study of both these properties.

The transport of a Brownian particle is always accompanied by a diffusive spread, and the quality of transport is affected by this diffusive spread. This property has been quantified via the ratio of current to the diffusion constant and is termed as the Péclet number, Pe . The Brownian particle takes a time $\tau = L/v$ to traverse a distance L with a velocity v and the diffusive spread of the particle in the same time is given by $\langle(\Delta q)^2\rangle = 2D\tau$. The criterion to have a reliable transport is that $\langle(\Delta q)^2\rangle = 2D\tau < L^2$. This implies that $Pe = Lv/D > 2$ for coherent transport. The Péclet numbers for some of the models like flashing and rocking ratchets show low coherence of transport with $Pe \sim 0.2$ and $Pe \sim 0.6$ [10], respectively. Experimental studies on molecular motors showed more reliable transport with Pe ranging from 2 - 6 [11]. Our earlier work on inhomogeneous ratchets in the presence of a single heat bath but, subjected to an external parametric white noise fluctuation, showed a coherent transport with Pe of the order of 3 [12]. From this and other works [13], one concludes that system inhomogeneities may enhance the effectiveness of transport, though sensitively

dependent on physical parameters.

The present paper is organised as follows. Section II gives the basic description of the systems, and also the analytical expressions for current and diffusion needed to evaluate the Péclet number. In Section III, we present detailed results for the dependence of current and quality of transport on system parameters. In Section IV, we conclude this paper with a brief summary.

II. MODEL

We begin with the equation of motion for a Brownian particle of mass m and position $x(t)$ coupled simultaneously with (a) an additive thermal noise bath at temperature T_A , and (b) a multiplicative noise bath having a spatially-varying friction coefficient $\eta(x)$ at temperature T_B . The particle moves in an underlying periodic potential $V(x)$. The equation of motion of the Brownian particle is given by [5, 6]

$$m\ddot{x} = -\Gamma(x)\dot{x} - V'(x) + \sqrt{\eta(x)}\xi_B(t) + \xi_A(t). \quad (2)$$

The Gaussian white noises $\xi_A(t)$ and $\xi_B(t)$ are independent, and obey the statistics:

$$\langle \xi_A(t) \rangle = 0, \quad \langle \xi_A(t)\xi_A(t') \rangle = 2\Gamma_A k_B T_A \delta(t-t'), \quad (3)$$

$$\langle \xi_B(t) \rangle = 0, \quad \langle \xi_B(t)\xi_B(t') \rangle = 2\Gamma_B k_B T_B \delta(t-t'). \quad (4)$$

The two noises together satisfy the fluctuation-dissipation theorem and $\Gamma(x) = \Gamma_A + \Gamma_B \eta(x)$. Here $\langle \dots \rangle$ denotes the ensemble average. In the present work, we have chosen $V(x) = V_0(1 - \cos x)$ and $\eta(x) = \eta_0[1 - \lambda \cos(x - \phi)]$. Here $0 < \lambda < 1$, and we set $\lambda = 0.9$ throughout for optimum values. The phase lag ϕ between $V(x)$ and $\eta(x)$ brings in asymmetry in the dynamics of the system. This inturn leads to an unidirectional current even in the presence of spatially periodic (nonratchet-like) potential.

When the friction term dominates inertia or on time-scales larger than the inverse friction coefficient, one can consider the overdamped limit of the Langevin equation. This corresponds to the adiabatic elimination of the fast variable (velocity) from the equation of motion by putting $\dot{p} = \ddot{x} = 0$. This approach is only applicable for a homogeneous system. For an inhomogeneous system, Sancho et al. [14] have given the proper prescription for the elimination of fast variables. The resultant overdamped Langevin equation for Eq. (2) is

given by [4]

$$\dot{x} = -\frac{V'(x)}{\Gamma(x)} - \frac{(\sqrt{\eta(x)})'\sqrt{\eta(x)}}{\Gamma^2(x)} + \frac{\xi_A(t)}{\Gamma(x)} + \frac{\sqrt{\eta(x)}}{\Gamma(x)}\xi_B(t). \quad (5)$$

The prime on a function denotes differentiation with respect to x . Using the van Kampen Lemma [15] and Novikov's theorem [16], we obtain the corresponding Fokker-Planck equation for the probability density $P(x, t)$ of a particle to be at point x at time t as follows:

$$\begin{aligned} \frac{\partial P(x, t)}{\partial t} = & \frac{\partial}{\partial x} \left\{ \frac{V'(x)}{\Gamma(x)} + \frac{T_B \Gamma_B}{\Gamma^2(x)} (\sqrt{\eta(x)})' \sqrt{\eta(x)} \right\} P + \frac{T_A \Gamma_A}{\Gamma(x)} \frac{\partial}{\partial x} \left[\frac{P}{\Gamma(x)} \right] \\ & + T_B \Gamma_B \frac{\sqrt{\eta(x)}}{\Gamma(x)} \frac{\partial}{\partial x} \left[\frac{\sqrt{\eta(x)}}{\Gamma(x)} P \right]. \end{aligned} \quad (6)$$

When the potential $V(x)$ is positive and unbounded, the system evolves to a steady-state distribution $P_s(x)$ characterised by zero current. Setting $J(x, t) = 0$ in Eq. (6), we obtain

$$P_s(x) = N \exp[-\psi(x)], \quad (7)$$

where

$$\psi(x) = \int^x dq \left[\frac{V'(q)\Gamma(q)}{T_A \Gamma_A + T_B \Gamma_B \eta(q)} + \frac{(T_B - T_A)}{\Gamma(q)} \frac{\Gamma_A \Gamma_B \eta'(q)}{T_A \Gamma_A + T_B \Gamma_B \eta(q)} \right]. \quad (8)$$

Here, $\psi(x)$ is the dimensionless effective potential, and N is the normalization constant.

For periodic functions $V(x)$ and $\eta(x)$ with periodicity 2π , a finite probability current is obtained. Following Risken [17], one readily gets the expression for the total probability current J as

$$J = \frac{[1 - \exp(-2\pi\delta)]}{\int_0^{2\pi} dy \exp[-\psi(y)] \int_y^{y+2\pi} dx \exp[\psi(x)]/A(x)}. \quad (9)$$

Here, δ determines the direction of current in the system and is given by

$$\delta = \psi(x) - \psi(x + 2\pi), \quad (10)$$

and $A(x)$ in Eq.(9) is given by

$$A(x) = \frac{\Gamma_A T_A + \Gamma_B T_B \eta(x)}{\Gamma^2(x)}. \quad (11)$$

From Eqs. (8) - (10), we can see that the system is in equilibrium when $T_A = T_B$, leading to zero net current. But when $T_A \neq T_B$, the system is rendered nonequilibrium and one can extract energy at the expense of increased entropy. It can also be seen that no current is possible when either Γ_A or Γ_B is absent. Again, if $\eta(x)$ is independent of x , there will be no net current flow in the system. When $T_A - T_B$ changes sign, the current also changes sign but not the magnitude.

One can also obtain an analytical expression for the diffusion constant D by following [18, 19] as

$$D = \frac{\int_{q_0}^{q_0+L} (dx/L) A(x) [I_+(x)]^2 I_-(x)}{\left[\int_{q_0}^{q_0+L} (dx/L) I_+(x) \right]^3} \quad (12)$$

where $I_+(x)$ and $I_-(x)$ are as follows:

$$I_+(x) = \frac{1}{A(x)} \exp[\psi(x)] \int_{x-L}^x dy \exp[-\psi(y)], \quad (13)$$

$$I_-(x) = \exp[-\psi(x)] \int_x^{x+L} dy \frac{1}{A(y)} \exp[\psi(y)]. \quad (14)$$

Here, L represents the period of the potential and is taken as 2π . From the above equations, the velocity ($v = 2\pi J$), diffusion constant (D) and the Péclet number (Pe) are studied as a function of different physical parameters. All the physical quantities are taken in dimensionless form. In particular, v and D are normalized by $(V_0/\eta_0 L)$ and (V_0/η_0) , respectively. Throughout our work we have set V_0 , η_0 and k_B to be unity. Similarly, Γ_A, Γ_B and T_A, T_B are scaled with respect to $V_0\eta_0$ and V_0 respectively. We have used the Gauss-Kronrod rules for numerical evaluations of the integrals involved [20].

III. DETAILED RESULTS AND DISCUSSION

In Fig. 1, we examine the behaviour of the effective potential $\psi(x)$ versus x , for two different values of ϕ . The parameter values are $T_A = 1$, $T_B = 0.1$, $\Gamma_A = 0.1$, $\lambda = 0.9$ and $\Gamma_B = 0.9$. For $0 < \phi < \pi$, the current is in the negative direction, while for $\pi < \phi < 2\pi$, the current is in the positive direction. This can be directly inferred from the slope of the potentials. The tilt in the effective potential identically vanishes when $\phi = 0$ or π . Hence it is expected that the unidirectional current does not arise for the case when the phase lag is 0 or π . In Fig. 1, we also study the effect of changing $\Gamma_B (= 0.1$ or $0.9)$ on $\psi(x)$ for a fixed $\phi = 0.3\pi$ value. We see that, as Γ_B increases, the tilt in effective potential increases. We also see from separate plots (not shown here) that the tilt is higher for smaller Γ_A values and also for higher temperature difference between the two baths. Hence, we set $T_A = 1.0$ and $T_B = 0.1$ throughout this paper unless specifically mentioned otherwise in the captions.

Next, let us study the behaviour of the probability current J , diffusion constant D and Péclet number Pe for various parameter values so as to extract an optimal set of parameters for coherent transport.

In Fig. 2 we plot J , D and Pe as a function of the phase difference ϕ for $\Gamma_A = 0.1$, and $\Gamma_B = 0.1, 0.9$. The current and diffusion constant varies periodically with ϕ , as expected. We find that an increase in Γ_B causes a decrease in J and D , thereby causing an increase in the Péclet number. We can see from the plot of Pe vs. ϕ that the transport is marginally coherent (~ 2) for a range of ϕ - values at the higher Γ_B - value.

For a particular value of phase difference ($\phi = 0.3\pi$), in Fig. 3 we plot J , D and Pe as a function of the temperature difference between the two baths, $T_A - T_B$. The other parameter values are $\Gamma_A = 0.1$ and $\Gamma_B = 0.9$. Here T_B is varied from 0 to 2 for a fixed $T_A = 1$. As expected, the current is zero when the temperatures of the two baths are the same. We also observe that the direction of current reverses depending upon the temperatures of the two baths A and B . For $T_B > T_A$, the current is in the negative direction and vice versa for $T_B < T_A$. Also, their magnitudes are different in both cases.

From Fig. 3, we also see that while the current exhibits a peak at $T_A - T_B \simeq 0.5$, D decreases with increasing $T_A - T_B$. On the other hand, Pe increases with increase in $T_A - T_B$, i.e., the transport goes towards the coherent regime.

In Fig. 4, we plot J , D and Pe as a function of T_B , for $\Gamma_A = 0.1$ and $\Gamma_A = 0.9$. The other parameter values are specified in the figure caption. For $\Gamma_A = 0.1$ we see $J \simeq 0$ in the presence of a single heat bath ($T_B \simeq 0$). As T_B is increased, the current starts to build up and shows a peaking behaviour. When the value of $T_B \rightarrow T_A$ there is no transport as expected. For a particular Γ_B value, this non-monotonous behaviour is seen only for lower values of Γ_A . When the value of Γ_A is increased beyond a critical value, there is a non-zero current even when the temperature of bath B is zero.

The plot of Pe vs. T_B in Fig. 4 shows that, as Γ_A is decreased, the Pe value goes up and $Pe \rightarrow 2$ for small T_B when $\Gamma_A = 0.1$. (We have shown here only two representative Γ_A - values). We also see that the Pe value is more stable for lower Γ_A values, i.e., $Pe \simeq 2$ up to some value of T_B , and then decreases with further increase in T_B . Thus, we conclude that $\Gamma_A \leq 0.1$ for higher transport coherence.

In Fig. 5 we plot J , D and Pe vs. Γ_B for $\Gamma_A = 0.1$ and 0.9 , $\phi = 0.3\pi$, $T_A = 1$ and $T_B = 0.1$. In this case, for $\Gamma_A = 0.1$, the current shows a peak with Γ_B , the diffusion constant decreases with increase in Γ_B and $Pe \rightarrow 2$ for $\Gamma_B \geq 0.3$. On increasing the Γ_A value, we see from separate plots (not shown here) that the values of J and D are reduced, but the value of Pe is almost the same, though $Pe > 2$ for much higher Γ_B values, say

$\Gamma_B = 5$. Thus, Fig. 5 also leads to the conclusion that a lower Γ_A - value along with a higher Γ_B - value aids transport coherence.

IV. SUMMARY AND DISCUSSION

Let us conclude this paper with a brief summary and discussion. We have studied the transport coherence of an overdamped Brownian particle in the presence of two thermal baths, namely A and B with different noise statistics. One of the baths, B , is characterized by the presence of a state-dependent friction coefficient. The system considered here is analogous to a simple model of a Maxwell-demon-type of engine, which extracts work out of the nonequilibrium state from thermal fluctuations by rectifying the internal fluctuations in the system [5, 6]. The space-dependent friction coefficient in bath B is necessary for generating unidirectional current in the absence of a bias. The direction of current (but not its magnitude) changes sign when $(T_A - T_B)$ changes sign. The current identically vanishes when the temperatures of both the baths are the same. Also, in the extreme high friction limit, the current vanishes as the particle cannot execute Brownian motion.

We have systematically analyzed the behaviour of current, diffusion and transport coherence as a function of system parameters. The problem of coherence of transport has not been addressed in the context of these systems. Our work demonstrates that a combination of lower Γ_A - value and a higher Γ_B - value would lead to an optimum transport coherence. Our study of the Péclet number shows that, for most of the parameter space, $Pe \leq 2$. Thus, we conclude from the present study that the transport is not coherent though it is possible to get high current.

Our study can be extended in several directions. For example, it would be interesting to study the efficiency of energy transduction in this Maxwell-demon-type heat engine by using the methods of stochastic energetics developed by Sekimoto [22]. The fact that the steady-state probability distribution $P_s(x)$, Eq. (7) is a nonlocal function of $V(x)$ and $\eta(x)$ itself can lead to much interesting physics and would form the basis of our future work.

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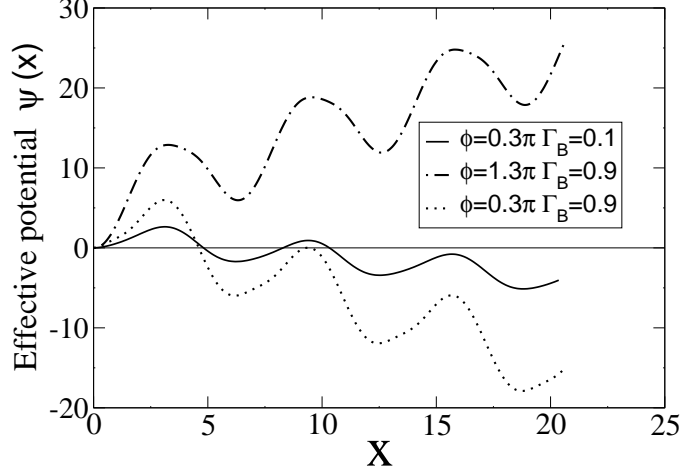


FIG. 1: Plot of $\psi(x)$ vs. x for the following parameter values. (a) $\Gamma_B = 0.9$ with $\phi = 0.3\pi$ and 1.3π , (b) $\Gamma_B = 0.1$ and 0.9 with $\phi = 0.3\pi$. The other parameter values are $T_A = 1$, $T_B = 0.1$ and $\Gamma_A = 0.1$.

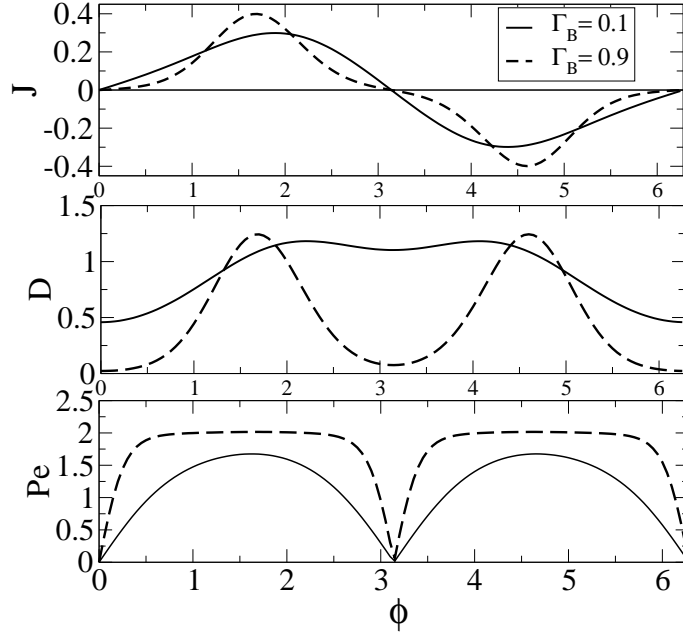


FIG. 2: Plot of J , D , Pe vs. ϕ for $\Gamma_A = 0.1$, and $\Gamma_B = 0.1$ and 0.9 . For $\Gamma_B = 0.9$, the quantities J and D are scaled up by a factor of 100 to make them comparable to the case $\Gamma_B = 0.1$.

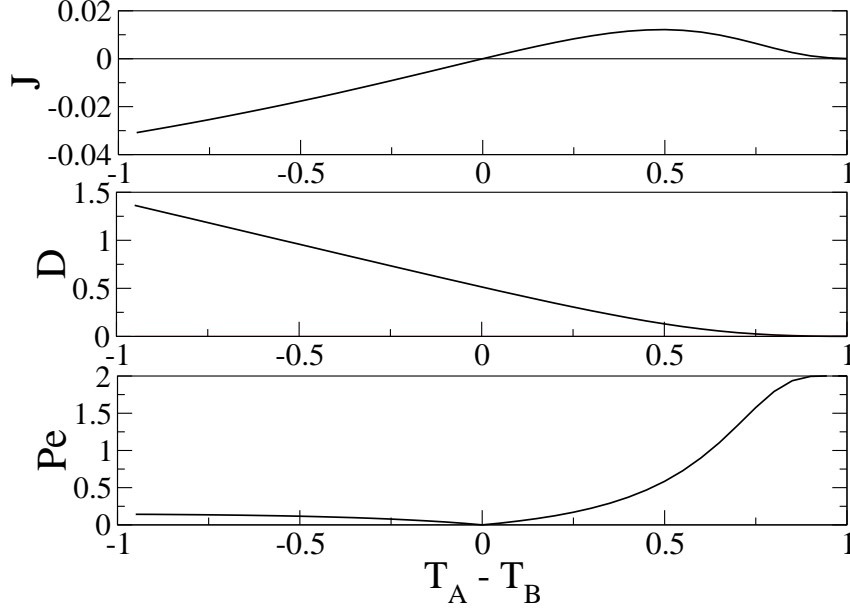


FIG. 3: Plot of J , D and Pe vs. $T_A - T_B$ for $\Gamma_A = 0.1$, $\Gamma_B = 0.9$, $\phi = 0.3\pi$. We set $T_A = 1$ and T_B varies from 0 to 2.

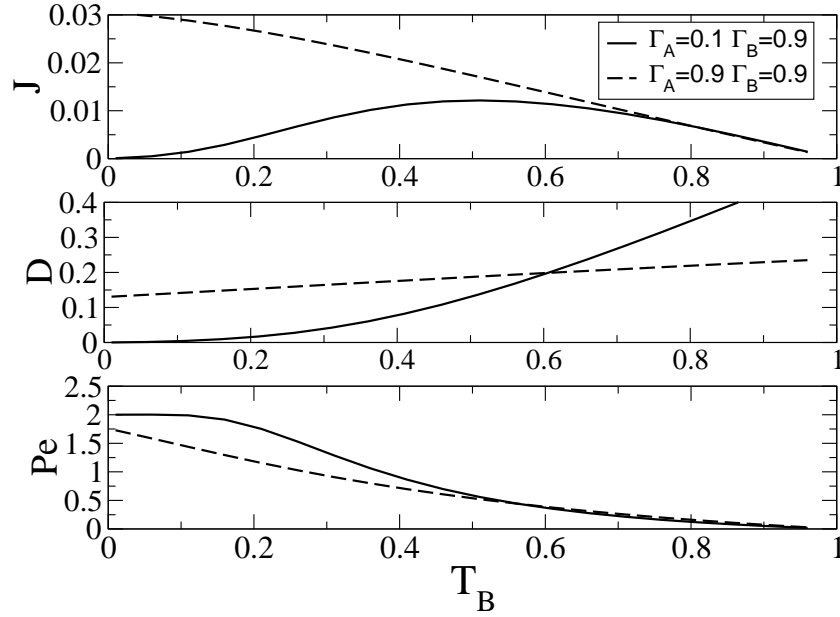


FIG. 4: Plot of J , D and Pe vs. T_B for $\Gamma_A = 0.1$ and 0.9 , $\Gamma_B = 0.9$, $\phi = 0.3\pi$, and $T_A = 1$.

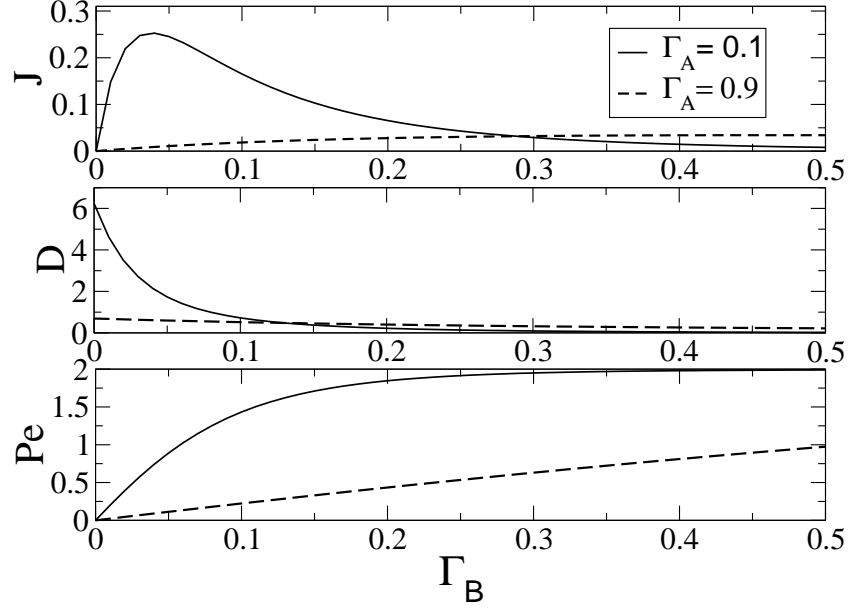


FIG. 5: Plot of J , D and Pe vs. Γ_B for $\Gamma_A = 0.1$ and 0.9 with $\phi = 0.3\pi$. The other parameter values are $T_A = 1$ and $T_B = 0.1$.