Giant diffusion and coherent transport in tilted periodic inhomogeneous systems.

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Abstract

We investigate the dynamics of an overdamped Brownian particle moving in a washboard potential with space dependent friction coefficient. Analytical expressions have been obtained for current and diffusion coefficient. We show that the effective diffusion coefficient can be enhanced or suppressed compared to that of the uniform friction case. The diffusion coefficient is maximum near the critical threshold ($F_c$), which is sensitive to temperature and the frictional profile. In some parameter regime we observe that increase in noise (temperature) decreases the diffusion, which is counter-intuitive. This leads to coherent transport with large mean velocity accompanied by small diffusion. This is shown explicitly by analysis of Péclet number, which has been introduced to study coherent or optimal transport. This phenomena is complementary to giant diffusion.

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I. INTRODUCTION

In recent times there has been a renewed interest in the study of transport properties of Brownian particles moving in periodic potential \[1\], with special emphasis on coherent transport and giant diffusion \[2, 3\]. The phenomenon of coherent or optimal transport is complimentary to the enhanced diffusion, wherein one is mainly concerned with transport currents with minimal dispersion or diffusion \[4\]. Compared to free diffusion coefficient (DC, \[D = k_B T/\gamma\]), DC is suppressed in the presence of periodic potential. However, in a nonequilibrium case i.e., in the presence of bias, it has been recently shown that DC can be made arbitrarily large (giant diffusion) compared to the bare diffusion, in the presence of periodic potential \[2\]. This enhancement at low temperature takes place near the critical threshold (at which deterministically running solution sets in). The reason for this enhancement has been attributed to the existence of instability between locked to running solution. In some cases enhancement by fourteen order of magnitude has been predicted, so that diffusion can be observed on a macroscopic scale at room temperature \[2\]. This enhancement decreases as we move away from the critical field in either direction. Exact result for DC in arbitrary potentials has been obtained in term of quadratures. In special cases an elegant simplification of quadrature have been carried out. Near the critical tilt, scaling behavior of DC for weak thermal noise has been obtained and different universality classes have been identified \[2\]. Approximate expression for DC in terms of mobility has been obtained earlier which deviates from the exact results near the critical threshold \[3\].

In a related development, study of coherent or optimal transport has been reported recently \[4\]. Coherent or optimal transport of Brownian particles refer to the case of large mean velocity accompanied with minimal diffusion. This can be quantified by dimensionless Péclet number (ratio of mean velocity to DC). The transport is most coherent when this number is maximum. The particle motion is mainly determined by two time scales; noise driven escape from potential minima over the barrier along the bias, followed by the relaxation into the next minima. The former depends strongly on temperature and the later weakly on the noise strength and has a small variance. It is possible to obtain coherent transport in the parameter regime at which the traversal time across the two consecutive minima in a washboard potential is dominated by the relaxational time. At optimal noise intensity certain regularity of the particle motion is expected which accounts for the maxi-
mum of Péclet number. In some cases (molecular separation devices) for higher reliability, one requires higher currents but with less dispersion (or DC) \[^{[3]}\]. This effect of coherent transport is related to the phenomenon of coherence resonance \[^{[6]}\] observed in excitable systems \[^{[4]}\].

In the present work we study both the mentioned phenomena in a space dependent frictional medium. For this we have considered a simple minimal model where the potential is sinusoidal and the friction coefficient is also periodic (sinusoidal) with the same period, but shifted in phase. Frictional inhomogeneities are not uncommon in nature. Here we mention a few. Brownian motion in confined geometries, porous media experience space dependent friction \[^{[7]}\]. Particles diffusing close to surface have space dependent friction coefficient \[^{[7, 8]}\]. It is believed that molecular motor proteins move close along the periodic structure of microtubules and will therefore experience a position dependent friction \[^{[9]}\]. Inhomogeneities in mobility (or friction) occurs naturally in super lattice structures and Josephson junctions \[^{[10]}\].

Frictional inhomogeneity changes the dynamics of the diffusing particle non-trivially, thereby affecting the passage times in different regions of the potential. However, it does not effect the equilibrium distribution. Thus thermally activated escape rates and relaxational rates within a given spatial period are affected significantly. This in turn has been shown to give rise to several counter-intuitive phenomena. Some of them are stochastic resonance in absence of external periodic drive \[^{[11]}\], noise induced stability in washboard potential \[^{[12]}\]. Single and multiple current reversals in adiabatic \[^{[13]}\] and nonadiabatic rocked system (thermal ratchets \[^{[14]}\]) respectively have also been reported \[^{[15]}\]. In these ratchet systems the magnitude of efficiency of energy transduction in finite frequency regime may be more than the efficiency in the adiabatic regime, i.e, quasistatic operation may not be efficient for conversion of input energy into mechanical work \[^{[16]}\]. All these above features are absent in the corresponding homogeneous case for the same simple potential.

In our present work we show that frictional inhomogeneities can give rise to additional new features in a tilted periodic potential. The observed giant enhancement of DC near the critical tilt can be controlled (enhanced or suppressed) in a space dependent frictional medium by suitably choosing the phase difference between the potential and the frictional profile. The most surprising feature is the noise induced suppression of diffusion, leading to coherent transport. Our results are based on analytical expressions for Péclet number and
DC in terms of moments of first passage times. In Section II we present our model and derive the expression for moments of first passage times. Using these, DC and Péclet number have been defined. In Section III A we analyze the nature of DC as function of system parameters, such as the applied external force and temperature. Section III B is devoted to the study of coherent or optimal transport in different regimes of parameter space. Finally in Section IV we present the summary of our findings.

II. MODEL

We consider an overdamped Brownian particle moving in a symmetric one-dimensional periodic potential $V_0(x)$ with space dependent friction coefficient $\eta(x)$ under the influence of constant external tilt $F$ at temperature $T$. For simplicity we take $V_0(x) = -\sin(x)$ and $\eta(x) = \eta_0(1 - \lambda \sin(x + 2\pi\phi))$, where $|\lambda| < 1$. $\phi$ determines the relative phase shift between friction coefficient and potential. The correct Langevin equation for such systems has been derived earlier from microscopic considerations [17] and is given by

$$\dot{x} = -\frac{V_0'(x) - F}{\eta(x)} - k_B T \frac{\eta'(x)}{(\eta(x))^2} + \sqrt{\frac{k_B T}{\eta(x)}} \xi(t),$$

where $\xi(t)$ is a zero mean Gaussian white noise with correlation $\langle \xi(t)\xi(t') \rangle = 2\delta(t - t')$. It should be noted that the above equation involves a multiplicative noise with an additional temperature dependent drift term which turns out to be essential for the system to approach correct thermal equilibrium state in absence of nonequilibrium forces [18].

The quantity of central interest in this work is the effective diffusion coefficient $D$ given by

$$D = \lim_{t \to \infty} \frac{\langle x^2(t) \rangle - \langle x(t) \rangle^2}{2t}.$$  

In the absence of potential, $D = \frac{k_B T}{\eta}$ (uniform $\eta$), is the usual Einstein relation. An exact analytical expression for $D$ and average current $J$ in terms of the moments of first passage time have been recently given [2, 4]. If the $n$-th moment of the first passage time from an arbitrary point $x_0$ to $b$ is given by $T_n(x_0 \to b) = \langle t^n(x_0 \to b) \rangle$, then

$$D = \frac{L^2}{2} \frac{T_2(x_0 \to x_0 + L) - [T_1(x_0 \to x_0 + L)]^2}{[T_1(x_0 \to x_0 + L)]^3}.$$  

(3)
For our problem (1), the moments of first passage time follow closed recursion relation (2, 19).
\[ T_n(x_0 \rightarrow b) = \frac{n}{D_0} \int_{x_0}^b dx \hat{\eta}(x) e^{\frac{V(x)}{k_B T}} \int_x^b dy e^{-\frac{V(y)}{k_B T}} T_{n-1}(y \rightarrow b), \] (4)
with \( T_0(y \rightarrow b) = 1 \). Here \( V(x) = V_0(x) - Fx \), \( D_0 = k_B T/\eta_0 \) and \( \hat{\eta} = \eta(x)/\eta_0 \). \( \eta_0 \) also happens to be the average value of friction coefficient over a period.

By using Eq. (3) and Eq. (4), and some straightforward algebra, we get
\[
D = D_0 \int_{x_0}^{x_0+L} dx I_\pm(x) I_\pm(x) I_\mp(x),
\] (5)
where,
\[
I_+(x) = \frac{1}{D_0} \hat{\eta}(x) e^{\frac{V(x)}{k_B T}} \int_{x-L}^x dy e^{-\frac{V(y)}{k_B T}}, \] (6a)
\[
I_-(x) = \frac{1}{D_0} e^{-\frac{V(x)}{k_B T}} \int_x^{x+L} dy \hat{\eta}(y) e^{\frac{V(y)}{k_B T}}. \] (6b)

The average current density \( J \) for this system has been derived earlier (12) which in term of Eqs. (5) is given by
\[
J = L \frac{1 - \exp(-LF/kT)}{\int_{x_0}^{x_0+L} dx I_\pm(x)}. \] (7)

The above expressions go over to the results obtained earlier for the case of space independent friction \( (\eta(x) = \eta_0, \lambda = 0) \) (2). It should be noted that Eqs. (3) are applicable when \( \eta(x) \) and \( V(x) \) have the same periodicity. Otherwise they have to be modified appropriately. We obtain results for DC by numerically integrating Eqs. (1) using a globally adaptive scheme based on Gauss-Kronrod rules. For the special case of \( V_0(x) = 0 \) we get
\[
D = D_0 \left( 1 + \frac{\lambda^2}{2} \left( \frac{1}{(k_B T)^2 + 1} \right) \right). \] (8)

We would like to mention here that in the absence of potential, DC explicitly depends on system inhomogeneities (via \( \lambda \)), however, steady current is independent of \( \lambda \) for the same case (12). \( F = 0 \) is the equilibrium situation and as expected \( D = D_0 \), which corroborates with the fact that frictional inhomogeneities cannot affect the equilibrium properties of the system. In the high temperature regime, \( D = D_0 \) as anticipated. For asymptotically large
field, DC saturates to a λ dependent value. This is solely attributed to space dependent friction. This somewhat surprising result also appears in the dependence of current on λ in the presence of potential and high field limit [13, 13].

In our subsequent analysis all the physical quantities are expressed in term of dimensionless units, DC is scaled with respect to $D_0$ or $V_0/\eta_0$ and $T$ is scaled with respect to $V_0$, where $V_0$ is half the potential barrier height (which is one). Period of the potential, $L = 2\pi$.

III. RESULTS AND DISCUSSIONS

A. Diffusion Coefficient

Though the system response to the applied field is generally given by the stationary current density $J = L < v >$, but this directed motion (or average position of the particle) is accompanied by dispersion due to the inherent stochastic nature of the transport. It has been shown previously that in a homogeneous medium this dispersion or diffusion becomes very large (giant enhancement of DC) near the critical tilt. This enhancement in DC can be order of magnitude larger than the bare DC in the absence of potential. We make a systematic study of this phenomena in the presence of system inhomogeneities. Though our parameter space is large, we restrict to a narrow relevant domain where we observe effects which are surprising, and arise due to system inhomogeneities.

![Diffusion Coefficient](image)

FIG. 1: Diffusion coefficient (5) vs $F$ for $\phi = 1.6\pi$. Inset shows the suppression of DC for inhomogeneous systems($\lambda = 0.9, \phi = 0.5\pi$, lower curve) as compared to the homogeneous systems.
In fig. 1 we plot DC as function of external tilt $F$ for different values of temperature $T$ ($\lambda = 0.9$ and $\phi = 1.6\pi$). It can be seen from the figure that DC exhibits a maxima as function of $F$. However, quantitative details depend sensitively on system parameters such as $\phi, T$ and $\lambda$. It can readily noticed from the curves A and B that DC has been enhanced by more than factor 2 as compared with the homogeneous case. On lowering the temperature the relative enhancement of DC still increases. DC can also be suppressed by properly tuning $\phi$. For $\phi = 0.5\pi$, DC near the critical field is suppressed by almost a factor 2 as compared to the homogeneous case (shown in the inset). Thus one can enhance or suppress DC near critical field by appropriately choosing the system parameters. It should be noted that in the case of enhancement, friction coefficient is lower on the immediate left side of the barrier and higher on the opposite side, where the relaxational motion takes place. When the frictional profile is opposite to the above case, suppression in DC occurs. When the phase difference between the two frictional profiles differ by $\pi$, then in one case enhancement and in the other suppression of DC can be observed as compared with the homogeneous case. Thus $\phi$ controls the fluctuations of first passage times, hence DC and current.

Unlike the behavior in the homogeneous case ($\lambda = 0$) where for small values of $T$ this peak value occur exactly at $F = 1$ (critical field), here the peak position is very sensitive to $\phi$ and can be shifted to either side of the bare critical field. Higher the temperature larger is the deviation from the critical threshold. Fig. 2 shows this behavior, where we have plotted

![Graph showing the force at which diffusion peaks ($F_p$) versus $\phi$ at $\lambda = 0.9$.](image)

**FIG. 2:** The value of $F$ at which $D/D_0$ peaks ($F_p$) versus $\phi$ at $\lambda = 0.9$.

the force at which diffusion peaks ($F_p$) as function of $\phi$ at $\lambda = 0.9$ for $T = 0.1$ and 0.01. For
$T = 0.1$ the peak can occur at as low as $F = 0.8$. The fact that $F = 0.8$ is away from critical threshold, hence enhancement in DC in this regime has to be attributed to space dependent friction. This is a clear example of system inhomogeneity affecting the dynamical evolution of the particle nontrivially. This will be discussed at the end of this section to explain many of our observations. We would also like to emphasize that critical threshold is not altered at temperature $T = 0$ for our present case as shown earlier [12].

Since with increasing tilt the barrier to forward motion decreases (thereby reducing the effect of exponential suppression of DC in the presence of periodic potential), therefore it is natural to expect that $D/D_0$ will increase with increasing $F$ (for $F < \text{barrier height}$). This is amply reflected in ref. [2], which corresponds to our $\lambda = 0$ case. In the presence of space dependent friction ($\lambda \neq 0$), $D/D_0$ can show a minimum (as shown in fig. 3) with increasing force (for $F < \text{critical field}$). This is surprising given the fact that current increases monotonically with increasing field (which we have checked separately) as expected. To observe this phenomena one has to properly choose the parameters. This is akin to the phenomena of coherent transport, wherein, increase in current is accompanied by decrease in DC. This we have discussed in detail in the later section as function of $T$, however, it is observed here as function of $F$ also.

Next we proceed to present the most interesting consequence of space dependent friction coefficient in our simple model. Unlike the expected result where the diffusion coefficient increases with temperature, here the diffusion can be suppressed by increasing the temperature. Fig. 4 highlights this. Here we have plotted $D$ as function of

![Fig. 3: $D/D_0$ vs $F$ for $\lambda = 0.9$ and $\phi = 0.84\pi$. The figure highlights the minima in DC with $F$.](image)

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FIG. 4: $D$ vs $k_B T$ for $\lambda = 0.9$ and $\phi = 1.4\pi$ and various values of $F$. The inset compares the variation of $D$ with $k_B T$ for $\lambda = 0.9$ with $\lambda = 0.0$. $F = 0.98$ in the inset.

$T$. $D$ is scaled with $V_0/\eta_0$ as mentioned in the Sec. II. For the inset we have taken $\phi = 1.36\pi$ and $1.44\pi$ at $F = 0.98$ and $\lambda = 0.9$. For homogeneous case ($\lambda = 0$), the minima is absent and $D$ increases monotonically with $T$. However, minima is clearly seen for the case $\lambda \neq 0$. The observed suppression occurs when $F$ is close to the critical field. In can be clearly seen from the figure that as we go away from the critical field the minima in DC shifts to higher values of temperature and importantly it becomes shallower. Below certain value of $F$, minima and hence the suppression of DC disappears. The existence of the suppression in DC is attributed to the competition between two time scales. First, noise driven escape over potential barrier from the minima along the bias and the second time scale being the relaxation into the next potential well from the barrier top [4]. It has been argued before that the second time scale is weakly dependent on noise strength and has a small variance as opposed to the first one. It is obvious that in transport processes when the second time scale dominates over the first it is expected to result in suppression of DC as function of noise strength (see for details ref. [4]). In the high temperature regime large thermal noise leads to large variance in the second time scale as the random motion of the particle both along and against the bias becomes equally important. Thus the DC increases as expected for higher temperatures, hence minima in DC. It is to be noted that for the case where $\phi = 1.4\pi$, the friction coefficient $\eta(x)$ is smaller near the barrier heights and moreover $F$
being close to critical threshold makes Arrhenius barrier crossing time scale (first time scale) smaller. As opposed to this, $\eta(x)$ is higher between the barrier height and the next potential minima along the bias thus slowing down the relaxation motion to the next minima. This naturally enhances the dominance of the relaxation time scale over the barrier crossing rate. This qualitatively explains our observed behaviour.

FIG. 5: The figure compares current, DC and Péclet number (from top to bottom) of the inhomogeneous system ($\lambda = 0.99$ and $\phi = 1.4\pi$, left hand side figures) with that of the homogeneous system ($\lambda = 0$, right hand side figures).

**B. Péclet number and coherent motion**

By coherent motion we mean large particle current with minimal diffusion. This property can be quantified by the dimensionless Péclet number $Pe$ defined as

$$Pe = \frac{L \langle \dot{x} \rangle}{D},$$

where $L \langle \dot{x} \rangle$ is the average current density $J$. The expression for the current density is given in Eq. (7). We make use of expressions (5 and 7) to calculate $Pe$. The parameter values
at which $Pe$ shows maxima correspond to the most coherent motion for that particular model. Higher the $Pe$ more coherent is the transport. It should be noted that the $Pe$ can show maxima though neither $J$ nor $D$ may show extrema. In fig. 3, we plot the current $J$, diffusion coefficient $D$ and the Péclet number $Pe$ (from top to bottom) for both space dependent (left column of fig. 3) and space independent friction (right column of fig. 3) cases. The average friction coefficient over a period in inhomogeneous case equals to the value taken for the homogeneous case. As pointed out earlier, though in the homogeneous case $J$ and $D$ is monotonic increasing function of $T$, the péclet number shows a maxima, the maximum value being very small compared to the space dependent friction case. For the chosen parameter values in the space dependent friction case, DC shows a minima with $T$ while the current increases monotonically. Moreover the magnitude of this current is larger than the corresponding current in the homogeneous friction case. This is indeed the most favorable condition of transport where increasing current is accompanied by decreasing DC. This is aptly reflected in the $Pe$, which shows enhancement (coherent motion or optimal transport) by an order of magnitude as compared with corresponding uniform friction case. The Péclet number is sensitively dependent on the phase factor $\phi$ and it can also be suppressed (diffusion dominates the transport) which we have not reported here. Hence we can control the degree of coherent motion.

IV. CONCLUSIONS

We have thus shown that both giant diffusion and coherent transport in a tilted periodic potential is sensitive to the frictional inhomogeneities of the medium. To analyze this problem we have taken a simple sinusoidal potential and periodic frictional profile with same periodicity but with a phase difference. Depending on the system parameters the value of DC near the critical threshold and Péclet number (indicating coherence in the transport) can be enhanced or decreased by an order of magnitude. Both these complimentary effects are important for practical applications. The regime where we observe the optimal transport is accompanied by decrease of DC with temperature, the aspect which is absent in the corresponding homogeneous case. We have focussed on a restricted parameter regime to highlight the most interesting results arising due system inhomogeneities, in systems with simple potential. It is known that in the present model depending on system parameters
current decreases with temperature, the effect akin to noise induced stability \[20\]. However, in this regime we have not observed any dramatic effect on DC as well as Péclet number. It is not clear whether noise induced stability (NIS) can enhance the coherence in the motion. The phenomenon of stochastic resonance (SR) in absence external ac field \[11\] is seen in this model. SR is characterized by the observation of peak in the particle mobility as function of system parameters such as $T$ and $F$ in certain parameter space. The analysis of Péclet number in this parameter space does not show any surprising features, so as to correlate with SR. This is due to the fact that SR occurs in the hight $T$ or high $F$ regime, where barriers to motion are absent. To observe the peak in the Péclet number the existence of barrier seems to be essential. To clarify the relation between SR, NIS and Péclet number one requires further detailed analysis.

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