Supersymmetry and Fokker-Planck dynamics in periodic potentials

Mamata Sahoo\textsuperscript{1}, Mangal C. Mahato\textsuperscript{2} and A. M. Jayannavar\textsuperscript{1}

\textsuperscript{1}Institute of Physics, Bhubaneswar-751005, India and

\textsuperscript{2}Department of Physics, North-Eastern Hill University, Shillong-793022, India

Abstract: Recently, the Fokker-Planck dynamics of particles in periodic potentials \( \pm V \), have been investigated by using the matrix continued fraction method. It was found that the two periodic potentials, one being bistable and the other metastable give the same diffusion coefficient in the overdamped limit. We show that this result naturally follows from the fact that the considered potentials in the corresponding Schrödinger equation form supersymmetric partners. We show that these differing potentials \( \pm V \) also exhibit symmetry in current and diffusion coefficients: \( J_+(F) = -J_-(-F) \) and \( D_+(F) = D_-(-F) \) in the presence of a constant applied force \( F \). Moreover, we show numerically that the transport properties in these potentials are related even in the presence of oscillating drive.

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Corresponding Author: A.M. Jayannavar

Email address: jayan@iopb.res.in
I. INTRODUCTION

Periodic potentials are common occurrences in diverse kinds of extended systems such as crystals in solids and microtubules in living systems. The nature of the potential profile depends on the medium and the particle moving through it. A Ag\textsuperscript{+} ion, for example, of a AgI crystal in the superionic phase\cite{1} moving in a certain direction may be gainfully modeled to encounter a periodic potential profile \( V(x) = A \cos kx + B \cos 2kx \) with two wavevector components instead of a simple cosinusoidal potential. Such potential profile modeling could be based on the consideration of crystal structure and the underlying energy landscape in the direction of motion of the ion. In some other direction, however, the periodic potential profile could be entirely different. The potential profile \( -V(x) \) is also periodic with the same periodicity as \( V(x) \) yet they have important differences. The potential \( V(x) \) is bistable in nature, whereas \( -V(x) \) has a metastable well within a period, Fig.1.

Recent studies show that an overdamped Brownian particle exhibits identical diffusive behavior in the potentials \( V(x) \) and \( -V(x) \) in the entire range of parameter \( \frac{A}{B} \) \cite{2}. However, the diffusion constant of underdamped Brownian particles are quite different for the two related potentials. In this work we reason and explain that this result follows from the fact that the potentials of the Schrödinger equation with (Eucldian time) corresponding to Fokker-Planck equation of motion \cite{3} with potentials \( \pm V(x) \) form supersymmetric pairs and hence have identical eigenvalue spectra\cite{4,5,6}. The identical eigenvalue spectra along with one to one correspondence between their eigenfunctions ensure that both the systems (i.e., with \( \pm V(x) \)) exhibit same long time average asymptotic behavior. This also implies that when a constant force \( F \) is applied to the potentials \( \pm V(x) \) the average stationary current will satisfy \( J_+(F) = -J_-(F) \) and the diffusion constant \( D_+(F) = D_-(F) \). This result can also be seen from the analytic solution of the Fokker-Planck equation. In addition, we show that when the system is driven periodically, both the potentials show similar diffusive behavior.
II. THE MODEL

Consider the motion of a particle moving in a tilted periodic potential \(V(x)\) and described by the overdamped Langevin equation\[3\]

\[
\gamma \frac{dx}{dt} = -\frac{\partial V(x)}{\partial x} + \xi(t),
\]

where the Gaussian random force \(\xi(t)\) satisfies \(\langle \xi(t) \rangle = 0\) and \(\langle \xi(t)\xi(t') \rangle = 2\gamma T \delta(t-t')\). Here \(\langle \ldots \rangle\) denotes thermal average at temperature \(T\) (written for \(k_B T\), where \(k_B\) is the Boltzmann constant). \(\gamma\) is the frictional drag coefficient. The corresponding Fokker-Planck equation (in dimensionless units) is written as \[3\]

\[
\frac{\partial P(x,t)}{\partial t} = L_{FP} P(x,t),
\]

where the Fokker-Planck operator \(L_{FP}\) is given by

\[
L_{FP} = \frac{\partial}{\partial x} (V'(x) + T \frac{\partial}{\partial x}).
\]

The prime over \(V(x)\) denotes derivative with respect to \(x\). After constructing the Hermitian operator \(L = e^{\Phi/2}L_{FP} e^{-\Phi/2}\), with the effective potential \(\Phi(x) = \frac{V(x)}{T}\), the time independent Schrödinger equation corresponding to the Fokker-Planck equation (2) can be written as \[3\]

\[
L \psi_n(x) = \left[ T \frac{\partial^2}{\partial x^2} - V_{S+}(x) \right] \psi_n(x)
\]

\[
L \psi_n(x) = -\lambda_n \psi_n(x)
\]

The Schrödinger eigenfunction \(\psi_n(x) = e^{-\Phi(x)/2} \phi_n(x)\), and the eigenvalues \(\lambda_n(\geq 0)\) are given by

\[
L_{FP} \phi_n(x) = -\lambda_n \phi_n(x)
\]

Here \(T\) substitutes for \(\frac{\hbar^2}{2m}\) in quantum mechanical Schrödinger equation. The Schrödinger potential \(V_{S+}(x)\) is obtained for the potential \(V(x)\) as

\[
V_{S+}(x) = -\frac{V''}{2} + \frac{V'^2}{4T}
\]
For the potential \(-V(x)\) the corresponding Schrödinger potential is
\[
V_{S-}(x) = \frac{V''}{2} + \frac{V'^2}{4T} \tag{8}
\]
The potentials \(V_{S\pm}(x) = W^2(x) \mp \sqrt{T} W'(x)\) constitute the supersymmetric partner potentials and \(W(x)\) is referred to as the superpotential in supersymmetric quantum mechanics literature. The superpotential \(W(x)\) can also be expressed in terms of the ground state wavefunction of the Hermitian operator \(L\) \cite{4}. For periodic potentials \(\pm V(x)\) in Fokker-Planck dynamics, it is known from supersymmetric quantum mechanics that the eigenvalue spectra (with energy bands and band gaps) of \(V_{S\pm}(x)\) of the corresponding Schrödinger equation in quantum mechanics are strictly isospectral and the eigenfunctions are directly related to each other being in one to one correspondence \cite{4}. The immediate implication of this observation is that the potentials \(\pm V(x)\) will exhibit identical transport behavior in the long time asymptotic limit. It is expected that the average or expectation values of all the dynamical variables for \(\pm V(x)\) will show similar behavior in the time asymptotic regime\cite{4}. In fact for a given potential \(V(x)\) in the presence of applied field \(F\) the analytic expressions for current, \(J\) and diffusion coefficient, \(D\), are given by\cite{7,8}
\[
J = 2\pi \frac{1 - \exp(-2\pi F/T)}{\int_{x_0+2\pi}^{x_0+2\pi} \frac{dx}{2\pi I_\pm(x)}} \tag{9}
\]
and
\[
D = D_0 \left| \int_{x_0}^{x_0+2\pi} \frac{dx I_\pm(x)}{\int_{x_0}^{x_0+2\pi} dx I_\pm(x)} \right|^3 \tag{10}
\]
where,
\[
I_+(x) = \frac{1}{D_0} e^{\frac{V(x)-Fx}{T}} \int_{x-2\pi}^{x} dy e^{-\frac{V(y)+Fy}{T}} \tag{11}
\]
\[
I_-(x) = \frac{1}{D_0} e^{-\frac{V(x)+Fx}{T}} \int_{x}^{x+2\pi} dy e^{\frac{V(y)-Fy}{T}} \tag{12}
\]
Here \(2\pi\) is the length of the period and \(D_0\) is the bare diffusion constant (= \(kT/\gamma\)). By tedious algebraic manipulation (for example see the appendix of ref \cite{7}) one can show that, for potentials \(\pm V(x)\), current \(J\) and diffusion coefficient \(D\), respectively, satisfy
the relations $J_+(F) = -J_-(F)$ and $D_+(F) = D_-(F)$. The subscripts $\pm$ refer to the potentials $\pm V(x)$. The result obtained in references [2] follows as a special case when $F = 0$, namely $D_+(F = 0) = D_-(F = 0)$.

III. RESULTS AND DISCUSSION

We have considered the potential $V(x) = A \cos kx + B \cos 2kx$ in the Langevin equation in equation (1) in its dimensionless form. We, in the following, as has been done from equation (2) onwards, measure energy in units of $A$, wavenumber in units of $k$ and the friction coefficient in units of $\gamma$ and all other variables are given in terms of combinations of $A$, $k$ and $\gamma$. Thus in these dimensionless units the potential reads as

$$V(x) = \cos x + B \cos 2x,$$

etc. Thus a particular choice of $B$ will fix the relative values of the two potential barriers. In a series of papers [2], the ratio of the diffusion constant to the bare diffusion constant ($D_0$) has been given in the entire range (0,1) of the ratios of the potential barriers of $V(x)$ in the overdamped as well as in the underdamped regime. In these works they calculate the diffusion coefficients by solving the Fokker-Planck equation (2) and (3) by the method of matrix continued fraction[3]. As mentioned in the previous sections their results in the high friction limit, can be understood from supersymmetric considerations as well as obtained from analytic expressions. We calculate in this work the diffusion constant $D$ and current $J$ in the presence of a constant force $F$. We calculate these quantities also for an asymmetric potential profile [fig.2]

$$V(x) = \cos x + \cos 2x + 0.25 \sin 3x.$$  

In the following the nature of currents $J$ and the diffusion constant $D$ calculated using expressions (9) and (10) respectively are presented.

Fig.3 shows the variation of current as a function of the constant applied force $F$ at temperature $T = 0.1$ for the symmetric potential $V(x) = \cos x + \cos 2x$. As
expected, for low values of $|F| \ll F_c$ (where the largest barrier to motion just disappears), the current effectively remains zero as the largest barrier height is much larger than $T = 0.1$ (at $F = 0$ the largest barrier height is 3.0). It may be noted that at temperature $T = 0$, there will be no current up to the critical field $F_c(\approx 2.74)$ as the particle will be in a locked state. Beyond $F_c$ the particle being in a running state leads to a finite current[3]. At finite temperature current begins to flow even before $F_c$ due to thermal activation. $J$ approaches its linear regime (mobility $\mu = 1$) soon after around $F$ equals 3. From the figure it is clear that $J_+(F) = -J_-(F)$ as also $J_+(F) = J_-(F)$, where the subscripts ($\pm$) on $J$ corresponds to the potentials $\pm V(x)$. Our results also corroborate the earlier obtained result that the diffusion constant acquires giant enhancement[7,8] at the critical field $F = F_c$ [inset of fig.3]. The giant enhancement in $D$ near $F_c$ is expected as a fall out of the instability between the locked state ($F < F_c$) and running state[7,8]. We also observe that both the potentials $\pm V(x)$ exhibit identical diffusive behavior $D_+(F) = D_-(F)$ for this symmetrical potential. In fig.4, we plot $J_\pm$ and $D_\pm$ for the periodic potential $\pm V(x)$, with $V(x) = \cos x + \cos 2x + 0.25 \sin 3x$, for the same temperature $T = 0.1$. Note that the critical field now have different values ($F_{c1} \approx -3.19$ and $F_{c2} \approx 2.12$) for different applied field directions. With the asymmetric potential we see that the relation $J_+(+F) = -J_-(F)$ is satisfied as mentioned in the introduction. $J(F)$ shows very similar behavior to what is shown in fig.3. The figure in the inset shows $D_+(F) = D_-(-F)$. For both the potentials the diffusion coefficient shows the resonant enhancement close to the corresponding critical fields $F_{c1}$ and $F_{c2}$. And the diffusion coefficient does show the symmetry with respect to $\pm F$, for either of the potentials $\pm V(x)$: $D(F) \neq D(-F)$, however, $D_+(F) = D_-(F)$.

So far we have considered the case for particle subjected to constant force. We now study particle subjected to ac forcing where particle probability density does not evolve to a steady state(rather it evolves to a time periodic state). It may be noted that supersymmetric arguments do not apply when time dependent forcings are included. However, even in this case we show numerically that diffusion constant shows the same
behaviour for potentials $\pm V(x)$. In Figs. 5 and 6 we plot the diffusion coefficient, as a result of an ac drive $F = A \cos(\omega t)$, as a function of $A$ at temperature $T = 0.25$. This is shown by solving the corresponding Langevin equation using Huen’s method[9]. The diffusion constant $D$ is obtained in the long time asymptotic limit as

$$D = \lim_{t \to \infty} \frac{1}{2t} [\langle x^2(t) \rangle - \langle x(t) \rangle^2]$$

Where $\langle ... \rangle$ denotes the ensemble averaging over a large number of trajectories. We discard the initial transients ($t_0 = 500\tau$) and allowed the system to evolve for $t = 25000\tau$. The time step $\tau$ is taken equal to 0.01 and 3500 ensembles are used to evaluate the averages (15).

In fig.5, we give the plot for the symmetric potential $V(x) = \cos x + \cos 2x$ for two frequencies $\omega = 1.0$ and $\omega = 10.0$ (inset). It is very clear from the figure that $D$ is same for both the potentials $\pm V(x)$ within our numerical accuracy. Also, for $\omega = 1.0$, $D$ shows a resonant behaviour at $3.0 < A < 4.0$. It should again be noted that the largest barrier height shown by the potential $V(x)$ equals 3.0. That is, peaking behavior is exhibited close to the extreme forcing equal to the critical static field $F_c$. This is where the particle has maximum likelihood of diffusing forward as well as in the backward direction thereby enhancing the diffusion coefficient. For amplitudes $A$ larger than about 3.0, the diffusion coefficients are larger than their bare diffusion coefficient values[7,8]. Thus this peak could be attributed to optimised enhancement of the escape rate by modulation for a given noise strength[9,10,11]. It will be interesting to see how the peaking behaviour of $D$ gets affected by the variation of temperature and frequency. For high frequency drive ($\omega = 10$, for example), however, the peak disappears completely (Inset, fig.5). Not only the peak disappears, the overall diffusivity itself gets reduced by about two orders of magnitude indicating that the particle excursion gets confined to a single well with only occasional jump to the right and left of the barriers, exhibiting same behaviour for both $\pm V(x)$. In fig.6, we plot the diffusion coefficient for the asymmetric potential $V(x) = \cos x + \cos 2x + 0.25 \sin 3x$ as a function of amplitude $A$ of the ac forcing $A \cos(\omega t)$ with $\omega = 1.0$ at temperature $T = 0.25$. This is shown by solving the corresponding Langevin equation using Huen’s method[9].
0.25. In this case too $D$ shows similar behavior to the symmetric potential case, fig.5. Remarkably, also for the asymmetric potential $D_+(A) = D_-(A)$.

IV. CONCLUSION

In conclusion, we have shown that the current and diffusion coefficients, in static potentials $\pm V(x)$ in the presence of constant force, are related by symmetry relations $J_+(F) = -J_-(F)$ and $D_+(F) = D_-(F)$, respectively. When the Fokker-Planck equation of motion is mapped on to the Schrödinger equation these potentials lead to supersymmetric Schrödinger partner potentials, whose eigenspectra are isospectral. Also, eigenfunctions are in one to one correspondence. Consequently, in the large time asymptotic limit these differing potentials give the stated behaviour of the transport coefficients. We have also shown, numerically, that in the presence of ac drive the diffusion coefficients exhibit same behaviour for $\pm V(x)$. This is surprising because supersymmetry arguments do not apply in the presence of time dependent fields. This, therefore, requires further investigation.

V. ACKNOWLEDGEMENT

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FIG. 1: The potentials $V(x) = \cos x + \cos 2x$ (solid line) and $-V(x)$ (dashed line) are plotted in dimensionless units for comparison.
FIG. 2: The potentials $V(x) = \cos x + \cos 2x + 0.25 \sin 3x$ (solid line) and $-V(x)$ (dashed line) are plotted in dimensionless units for comparison.
FIG. 3: The currents $J_{\pm}$ and (inset) $D_{\pm}$ are plotted as a function of constant applied force $F$ for symmetric potentials. The subscripts $\pm$ refer to the potentials $\pm V(x)$ and at temperature $T = 0.1$. Results for $\pm V(x)$ are identical.
FIG. 4: The currents $J_\pm$ and (inset) $D_\pm$ are plotted as a function of constant applied force $F$ for asymmetric potentials. The subscripts $\pm$ refers to the potentials $\pm V(x)$ and at temperature $T = 0.1$. Continuous lines correspond to $+V(x)$. 
FIG. 5: The diffusion constants $D_{\pm}$ are plotted as a function of the amplitude $A$ of ac force for the symmetric potential $\pm V(x)$ at frequencies $\omega = 1.0$ and (inset) $\omega = 10.0$ and at temperature $T = 0.25$. The continuous line corresponds to $D_+$. 
FIG. 6: The variation of $D_{\pm}$ as a function of amplitude $A$ of a ac drive for the asymmetric potential $\pm V(x)$, (eq.(14)) at temperature $T = 0.25$ and high frequency $\omega = 1.0$. Continuous line for $+V(x)$. 