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A field-theoretical approach to one-dimensional Brownian motion in a cosine potential

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Abstract. One-dimensional (1D) Brownian motion in a cosine potential for the case of weak noise is considered quantitatively. The probability distribution of the motion is derived through the 'instanton' treatment of quantum field theory under some assumptions. This approach leads to a convenient form of the probability distribution for the calculation of the mean-squared deviation and/or the effective diffusion constant. Comparison with numerical simulations is reported.

1. Introduction

Brownian motion is that undergone by a particle in a thermal reservoir. This motion is modelled by considering the particle to be subject to a stochastic noise force. Because of the randomness of the noise, the position of the particle is described by a probability distribution that the particle is within a given position interval at a given time when the original position is specified.

There are several examples in which the probability distributions are exactly known [1]. One of these is, of course, the Brownian motion of a free particle. In this case, the particle can run away anywhere as the observation time tends to infinity. Another well known example is the so-called Ornstein–Uhlenbeck process, describing the stochastic motion of a particle subject to a harmonic potential in a viscous medium. In this process, the mean deviation of the particle is always finite however long we may observe; the motion is confined around the minimum of the harmonic potential. The reason for this confinement is obvious. In a harmonic potential, the further the particle moves from the minimum, the stronger is the force which brings the particle back.

Motion in a 1D cosine potential has, in some sense, an intermediate nature between that of the free particle and that in a harmonic potential. Here, the potential has multiple minima, and the direction of the force changes periodically. When the particle is near a minimum, the potential to which the particle is subject is almost harmonic, and the particle is pulled back to the original minimum. Thus, if we observe the motion locally, it is similar to that of the Ornstein–Uhlenbeck process. However, when the particle moves a distance equal to half the period of the potential, the direction of the force changes, and the particle tends to be pulled toward the next minimum. Thus, if we see the motion globally, the particle can diffuse to any distance from the original minimum as the observation time tends to infinity. In other words, the universality class of the motion is that of Brownian motion of a free particle. The effective diffusion constant is, however, much reduced from the original one because of the pull-back force. When the 'bare' diffusion constant is sufficiently small, the particle will remain at the original minimum even after a very long time. In such cases, the motion is effectively confined to one particular minimum during some characteristic time. The characteristic time may be so long that, in the application to real problems, the diffusive nature of the motion does not appear during a practical observation time.

In order to clarify this point, a quantitative study of the probability distribution of this motion is needed. There are, of course, many studies on Brownian motion in a periodic potential [2]. To the best of our knowledge, however, no convenient form of the probability distribution of Brownian motion in a genuine cosine potential can be found in the literature, even under approximations.

In this paper, we treat the probability distribution of this system to fill this gap. We proceed as follows. In section 2, the probability distribution of the motion for the case of weak noise is derived. In the derivation, a functional integral approach is used. As far as we know, there is no previously existing explicit use of this approach for the consideration of the probability distribution of the system in question. Using this result, the mean-squared deviation and the effective diffusion constant are calculated. In section 3, the qualitative and quantitative picture of this Brownian motion is described. In addition, the comparison of these results with numerical simulations is reported. The technical details of the calculation in section 2 are included in appendices.

2. Derivation of the probability distribution and the effective diffusion constant

The system of interest is described by the following Langevin equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}q(t) = -\beta \sin q(t) + \nu(t) \tag{1}$$

where $q(t)$ is the position of a particle at time t; β is the height of the potential, and $\nu(t)$ is a 'white noise' force. The time–time correlation of this noise force is given by the equation

$$\langle \nu(t)\nu(t')\rangle = 2D\delta(t-t') \tag{2}$$

where D is the diffusion constant of the system, and $\delta(x)$ is the Dirac delta function. We rewrite (1) and (2), rescaling time to obtain the following equations:

$$\frac{\mathrm{d}}{\mathrm{d}\tau}q(\tau) = -\sin q(\tau) + \nu(\tau) \tag{3}$$

and

$$\langle \nu(\tau)\nu(\tau')\rangle = 2\alpha\delta(\tau-\tau') \tag{4}$$

where $\tau(\equiv \beta t)$ is the dimensionless time, and $\alpha(\equiv D/\beta)$ is the dimensionless diffusion constant. In the following, the terms 'time' and 'diffusion constant' will always denote these dimensionless quantities.

Our concern is the probability distribution $P(q, T)$ that the particle is in a given position interval $(q, q+\mathrm{d}q)$ at a given time T. We take the position at $T = 0$ to be $q = 0$. Generally speaking, in the study of probability distributions of stochastic processes, it is common to consider the Fokker–Planck equation of the system with suitable boundary conditions. In this case, the Fokker–Planck equation is

$$\frac{\partial}{\partial \tau}P(q,\tau) = \alpha\frac{\partial^2}{\partial q^2}P(q,\tau) + \frac{\partial}{\partial q}\left(\sin q P(q,\tau)\right) . \tag{5}$$

It is very difficult, however, to solve this differential equation analytically.

Rather than attempting to solve this Fokker–Planck equation directly, we take another approach. It is known that the solution of the differential equation (5) is formally expressed in the functional integral representation [3]

$$P(q,T) = \mathcal{N}\int \mathcal{D}q(\tau)\exp\left(-\frac{S[q(\tau)]}{2\alpha}\right) \tag{6}$$

where the 'action' functional is

$$S[q(\tau)] = \int_{-T/2}^{T/2} \mathrm{d}\tau\, L[q(\tau)] \tag{7}$$

with the 'Lagrangian'

$$L[q(\tau)] = \frac{1}{2}\left[\left(\frac{\mathrm{d}}{\mathrm{d}\tau}q(\tau) + \sin q(\tau)\right)^2 - 2\alpha\cos q(\tau)\right]. \tag{8}$$

$\mathcal{N}$ in (6) is a normalization constant. The functional integration is taken over the set of all paths which satisfy the boundary condition that the particle is at the origin when $\tau = -T/2$ and at the position q when $\tau = T/2$. Notice that for convenience we have redefined the origin of time.

Even in this representation, it is very difficult to perform this integration under the most general conditions. We therefore confine our interest to the case of a small diffusion constant of the order unity or smaller and long observation time of the order 10^4 or more. As stated in the introduction, this case is of interest in this paper. In addition, we make the following argument in order to simplify the form of the probability distribution from a physical point of view. As described in the introduction, the motion near each potential minimum is almost the same as that of the Ornstein–Uhlenbeck process when the diffusion constant is small. The Ornstein–Uhlenbeck process has the following normalized stationary probability distribution:

$$P_{\mathrm{OU}}(q;q_0) = \frac{1}{\sqrt{2\pi\alpha}}\mathrm{e}^{-(q-q_0)^2/2\alpha} \tag{9}$$

in our units; q_0 is the position of the potential minimum. We assume that the probability distribution in a cosine potential can be decomposed in the following form:

$$P(q,T) = \sum_n P_{2n\pi}(\alpha,T)P_{\mathrm{OU}}(q;2n\pi) \tag{10}$$

where n is an integer. The normalization condition becomes

$$\sum_n P_{2n\pi}(\alpha,T) = 1 \tag{11}$$

since $P_{\mathrm{OU}}(q;2n\pi)$ is already normalized. $P_{2n\pi}(\alpha,t)$ can be interpreted as the discretized probability that the position of the particle falls within one particular sector $((2n-1)\pi, (2n+1)\pi)$ after a long time T for a small diffusion constant α. The boundary condition for the evaluation of $P_{2n\pi}(\alpha,T)$ is that $q=0$ at $\tau=-T/2$ and $q=2n\pi$ at $\tau=T/2$.

In this case, we can use the 'instanton' treatment of quantum field theory for the evaluation of the functional integral. When α is sufficiently small, the functional integral in (6) is almost completely governed by the paths which give the extrema of the action. Such paths satisfy the Euler–Lagrange equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\,q(\tau) = \sin q(\tau)\cos q(\tau) + \alpha\sin q(\tau). \tag{12}$$

The trivial solution is the stationary solution, $q(\tau) = 2n\pi$. But this path does not contribute to the probability $P_{2n\pi}(\alpha,T)$ when $n\neq 0$. The important solution for our problem is the

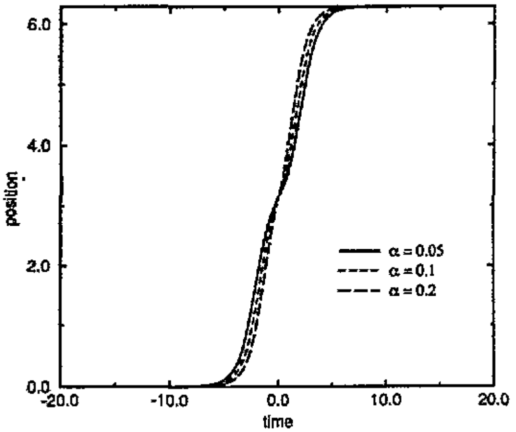

Figure 1. Shapes of instantons for three values of α. The 'jump' time at which each instanton passes through the potential maximum π is chosen to be zero.

'instanton' solution. This solution satisfies the boundary condition that the position at $\tau = -\infty$ is $2n\pi$ and that the position at $\tau = +\infty$ is $2(n \pm 1)\pi$. The solution with the positive sign is called an instanton, and that with the negative sign is called an anti-instanton. At an arbitrary time during this interval, the particle at a given minimum 'instantaneously' tunnels through the potential barrier to the next minimum. From the direct integration of (12), we can obtain the implicit expression of the instanton solution

$$\tau - \tau_0 = \int_{(2n+1)\pi}^{q} \frac{\mathrm{d}\tilde{q}}{\sqrt{\sin^2 \tilde{q} + 4\alpha \sin^2(\tilde{q}/2)}} \tag{13}$$

where τ_0 is the time when the particle passes the maximum of the potential. We call this τ_0 the 'jump' time. q takes a value between $2n\pi$ and $2(n+1)\pi$. This integration can be performed analytically, and we have

$$\tau - \tau_0 = \frac{1}{4\sqrt{1+\alpha}} \log \frac{\left(\sqrt{(1+\alpha)\left(\alpha + u_0^2\right)} + u_0\right)^2 - \alpha^2}{\left(\sqrt{(1+\alpha)\left(\alpha + u_0^2\right)} - u_0\right)^2 - \alpha^2} \tag{14}$$

with

$$u_0 = \cos(q/2) \qquad 2n\pi \leqslant q \leqslant 2(n+1)\pi\,. \tag{15}$$

The shapes of the instantons are shown in figure 1 for several values of α. The order of the 'width' of these instantons are about ten in our unit for the values of α in interest.

Using these 'instantons', we can perform the functional integration in (6). Although the calculation is fairly standard [4], we describe it briefly for the sake of completeness. Each path which contributes to this calculation starts from the origin at $\tau = -T/2$ and reaches the position $2n\pi$ at $\tau = T/2$. Between these times the particle can go anywhere. Now, the diffusion constant α is very small and the observation time T is very long by assumption. In this case, the important paths are arbitrary connections of m-instantons and $\bar{m}$-anti-instantons which satisfy the relation $m - \bar{m} = n$. In figure 2, we show an example of such paths.

Before proceeding with the evaluation of the functional integral, we should note that the following calculation is based on the so-called dilute gas approximation, in which it is assumed that the distance between each instanton is large compared to the width of one instanton. This assumption is justified because the observation time $T \sim \mathrm{O}(10^4)$ is very large compared to the width of the instantons ($\sim \mathrm{O}(10)$). A more detailed account of the validity of this approximation can be found in the next section.

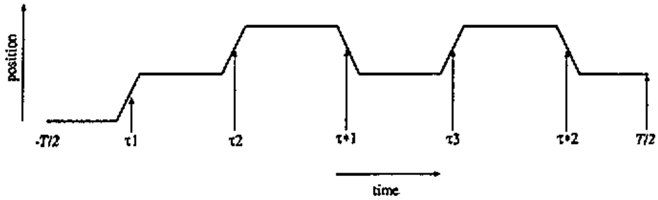

Figure 2. An example of the path which contributes to $P_{2\pi}$. This path consists of three instantons and two anti-instantons. The 'jump' times of instantons are denoted as $\tau 1, \tau 2, \tau 3$ and that of anti-instantons as $\tau^* 1, \tau^* 2$.

In the dilute gas approximation, the width of an (anti-)instanton is considered to be infinitesimal. The contribution from one particular path (e.g. the one in figure 2) consists of the following factors.

(i) Since the locations of each instanton in the interval $(-T/2, T/2)$ are arbitrary, there is a factor due to the integration over the location of the centre of the m instantons:

$$\int_{-T/2}^{T/2} \mathrm{d}t_1 \int_{-T/2}^{t_1} \mathrm{d}t_2 \cdots \int_{-T/2}^{t_{m-1}} \mathrm{d}t_m = \frac{T^m}{m!}. \tag{16}$$

Similarly, the factor from the $\bar{m}$ anti-instantons is $T^{\bar{m}}/\bar{m}!$.

(ii) From each (anti-)instanton, there is a factor due to the action of a single (anti-)instanton, which we denote as S_0. We have

$$S_0 = 4\left(\sqrt{1+\alpha} + \alpha \log \frac{1+\sqrt{1+\alpha}}{\sqrt{\alpha}}\right) \tag{17}$$

after an elementary calculation (see appendix A).

For the m-instanton and $\bar{m}$-anti-instanton path, the factor due to this action is

$$\left[\exp\left(-\frac{S_0}{2\alpha}\right)\right]^{m+\bar{m}}. \tag{18}$$

(iii) Finally, we include the harmonic fluctuations around the path. One instanton path is almost straight except in the vicinity of the 'jump' time. In figure 3, we show three time regions in an instanton path in the time interval $(-t/2, t/2)$. The 'jump' time is t_0. In the regions t_{I} and t_{III}, the path is considered to be straight. Since the region t_{II} is infinitesimal compared to the whole interval, the factor due to the fluctuations around this path can be written as

$$(\text{fluctuation around a straight line}) \times K = \frac{(1+\alpha)^{1/4}}{\sqrt{4\pi\alpha}} \mathrm{e}^{-t\sqrt{1+\alpha}/2} \frac{4}{\sqrt{2\pi}} \frac{(1+\alpha)^{5/4}}{\alpha} \tag{19}$$

where K is a correction factor from the contribution from the region t_{II}. For a detailed description of the calculation of K, see appendix B. To sum up, the factor due to the harmonic fluctuations for the m-instanton and $\bar{m}$-anti-instanton path is

$$\frac{(1+\alpha)^{1/4}}{\sqrt{4\pi\alpha}} \mathrm{e}^{-T\sqrt{1+\alpha}/2} K^{m+\bar{m}}. \tag{20}$$

Up to now, the contribution from one particular path is

$$\frac{(1+\alpha)^{1/4}}{4\pi\alpha} \mathrm{e}^{-T\sqrt{1+\alpha}/2} \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\right)^m}{m!} \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\right)^{\bar{m}}}{\bar{m}!}. \tag{21}$$

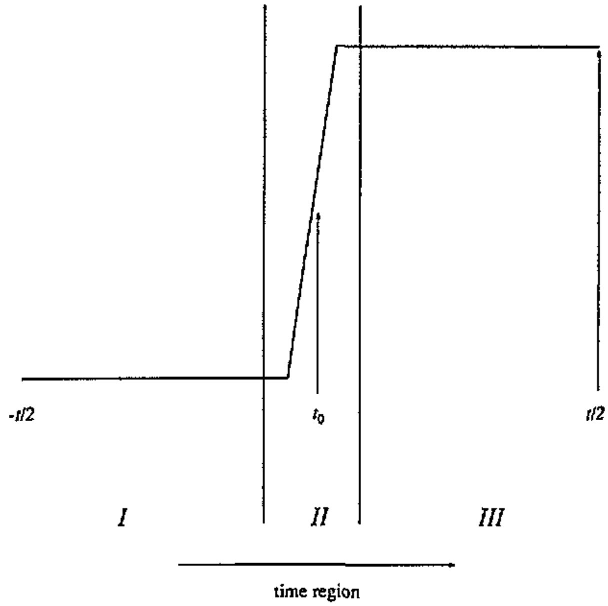

Figure 3. Three time regions of an instanton. In regions I and III, the path is almost straight. A significant contribution of fluctuations different from a straight line comes from region II.

After summing up all the contributions from the paths which satisfy the condition $n = m - \bar{m}$, we have the expression for $P_{2n\pi}(\alpha, T)$, which is

$$P_{2n\pi} = (n\text{-independent factor}) \sum_{m,\bar{m}} \delta_{m-\bar{m},n} \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\right)^m}{m!} \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\right)^{\bar{m}}}{\bar{m}!} \tag{22}$$

where $\delta_{i,j}$ is the Kronecker δ symbol.

With the help of the identity

$$\delta_{m-\bar{m},n} = \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \mathrm{e}^{\mathrm{i}\theta(m-\bar{m}-n)} \tag{23}$$

we can calculate $P_{2n\pi}(\alpha, T)$ as

$$\begin{aligned} P_{2n\pi} &\propto \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \mathrm{e}^{-\mathrm{i}\theta n} \sum_m \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\mathrm{e}^{\mathrm{i}\theta}\right)^m}{m!} \sum_{\bar{m}} \frac{\left(KT\mathrm{e}^{-S_0/2\alpha}\mathrm{e}^{-\mathrm{i}\theta}\right)^{\bar{m}}}{\bar{m}!} \\ &= \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \mathrm{e}^{-\mathrm{i}\theta n} \exp\left[KT\mathrm{e}^{-S_0/2\alpha}\left(\mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta}\right)\right] \\ &= \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \mathrm{e}^{-\mathrm{i}\theta n} \exp\left(2KT\mathrm{e}^{-S_0/2\alpha} \cos\theta\right) \\ &= I_n(z(\alpha, T)) \end{aligned} \tag{24}$$

with the argument $z(\alpha, T)$, which is the dimensionless time-scale of the motion

$$z(\alpha, T) = 2KT\mathrm{e}^{-S_0/2\alpha} \tag{25}$$

$$= 4\sqrt{\frac{2}{\pi}} \frac{(1+\alpha)^{5/4}}{\alpha} T \exp\left[-\frac{2}{\alpha}\left(\sqrt{1+\alpha} + \alpha \log \frac{1+\sqrt{1+\alpha}}{\sqrt{\alpha}}\right)\right]. \tag{26}$$

$I_n(z)$ is the modified Bessel function of the nth order. Notice that the dependence of this time-scale $z(\alpha, T)$ on α is highly non-analytic for small α. In other words, this result cannot be obtained through a perturbative approach.

For normalization, the identity

$$e^z = I_0(z) + 2I_1(z) + 2I_2(z) + \cdots \tag{27}$$

is useful [5]. Using this identity, we obtain the normalized probability distribution:

$$P_{2n\pi}(\alpha, T) = I_n(z(\alpha, T)) \exp(-z(\alpha, T)) . \tag{28}$$

This is the first result of this paper.

The next important quantity of the motion is the mean-squared deviation as a function of observation time. Now that we have the probability distribution, we can calculate this quantity as follows:

$$\begin{aligned}
\langle q^2 \rangle &= \int_{-\infty}^{\infty} dq\, q^2 \left[\sum_{n=-\infty}^{\infty} e^{-z} I_n(z) \frac{1}{\sqrt{2\pi\alpha}} e^{-(q-2n\pi)^2/2\alpha} \right] \\
&\cong \sum_n e^{-z} I_n(z) \int_{-\infty}^{\infty} dq\, q^2 \frac{1}{\sqrt{2\pi\alpha}} e^{-(q-2n\pi)^2/2\alpha} \\
&= \sum_n e^{-z} I_n(z) \int_{-\infty}^{\infty} d\tilde{q}\ (\tilde{q} + 2n\pi)^2 \frac{1}{\sqrt{2\pi\alpha}} e^{-\tilde{q}^2/2\alpha} \\
&= \sum_n 4n^2\pi^2 e^{-z} I_n(z) + \sum_n e^{-z} I_n(z) \int_{-\infty}^{\infty} d\tilde{q}\, \tilde{q}^2 \frac{1}{\sqrt{2\pi\alpha}} e^{-\tilde{q}^2/2\alpha} \\
&= 4\pi^2 e^{-z} \sum_{n=-\infty}^{\infty} n^2 I_n(z) + \alpha .
\end{aligned}$$

In order to calculate the first term, we use the identity [5]

$$e^{z\cos\theta} = I_0(z) + 2\sum_{n=1}^{\infty} I_n(z) \cos n\theta . \tag{29}$$

After taking the derivative with respect to θ twice, we set $\theta = 0$, and we have

$$\begin{aligned}
ze^z &= 2\sum_{n=1}^{\infty} n^2 I_n(z) \\
&= \sum_{n=-\infty}^{\infty} n^2 I_n(z) .
\end{aligned} \tag{30}$$

Thus, the mean-squared deviation becomes

$$\langle q^2 \rangle = 4\pi^2 z + \alpha . \tag{31}$$

Since $z = 2KTe^{-S_0/2\alpha}$,

$$\langle q^2 \rangle = 4\pi^2 2KTe^{-S_0/2\alpha} + \alpha . \tag{32}$$

Therefore, after a long time, the mean-squared deviation is almost proportional to the observation time; in other words, the long time behaviour of the motion is indeed that of the free diffusion.

The effective diffusion constant of the motion is well defined

$$
\begin{aligned}
\alpha_{\rm eff} &= \lim_{T\to\infty} \frac{\langle q^2\rangle}{2T} \\
&= 4\pi^2 K \mathrm{e}^{-S_0/2\alpha} \\
&= 8\pi\sqrt{2\pi}\frac{(1+\alpha)^{5/4}}{\alpha} \exp\left[-\frac{2}{\alpha}\left(\sqrt{1+\alpha}+\alpha\log\frac{1+\sqrt{1+\alpha}}{\sqrt{\alpha}}\right)\right].
\end{aligned}
\tag{33}
$$

This is the second result of this paper.

3. Discussion and conclusion

First, we argue the validity of the dilute gas approximation. In the dilute gas approximation, it is assumed that the instantons or anti-instantons on each path are well separated. This means that the important paths in the summation in (22) are those of which the density of instantons or anti-instantons is small. For any fixed x, the terms in the exponential series, $\sum_n x^n/n!$, grow with n until n is of the order of x, and after this point, they begin to decrease rapidly. Applying this to the sum in (22), we see that the important values of m are those for which $m \sim KT\mathrm{e}^{-S_0/2\alpha}$. Thus, the important density of the instantons in the summation in (22),

$$
\frac{m}{T} \sim K\mathrm{e}^{-S_0/2\alpha} \tag{34}
$$

depends only on α. For $\alpha = 0.1$, $K\mathrm{e}^{-S_0/2\alpha} \cong 3.3\times10^{-10}$, This value increases monotonically with α. For $\alpha = 0.5$, $K\mathrm{e}^{-S_0/2\alpha} \cong 3.9\times10^{-3}$. Therefore, the dilute gas approximation is valid for values of α of interest.

Next, we proceed to the qualitative and quantitative discription of Brownian motion in a cosine potential using the probability distribution derived in the previous section.

In figure 4, we plot the effective diffusion constant (33) as a function of the 'bare' diffusion constant α. The plot is for $0.15 \leqslant \alpha \leqslant 0.20$. For comparison, we also show in this figure two sequences of data obtained by direct sampling of the Langevin equation (1). For each data point, we took the mean-squared deviation $\langle q^2\rangle$ of 1000 samples after a running time $T = 3\times10^4$. The diffusion constants were calculated as $\langle q^2\rangle/2T$. For $\alpha < 0.15$, the mean-squared deviation is of the order of the bare diffusion constant α, and does not increase during the running time of the simulations. For $\alpha \leqslant 0.17$, the fittings are satisfactory, and we may say that for such values (33) describes the nature of the motion well. For $\alpha > 0.17$, the deviation of the theoretical values from the data obtained by simulations becomes larger. This manifests the invalidity of the saddle-point evaluation of the functional integration. Note that the theoretical values are always larger than those found from simulations. This means that the value obtained from (33) can be used as an upper bound of the effective diffusion constant for any values of α.

Next, we consider the time evolution of the position of the particle.

As described in the previous section, the qualitative nature of the motion is that of the free particle diffusion. In other words, the particle can always escape from the original minimum however small the diffusion constant is. In many cases of the application to real problems, however, there is an intrinsic time-scale of the system, and the situation that the motion is effectively confined to the original minimum within this time-scale can occur.

Using the expression of the mean-squared deviation (32), we can define the characteristic time T^*_α as the value at which the relation

$$
\langle q^2\rangle = 4\pi^2 2KT^*_\alpha \mathrm{e}^{-S_0/2\alpha} + \alpha = 4\pi^2 \tag{35}
$$

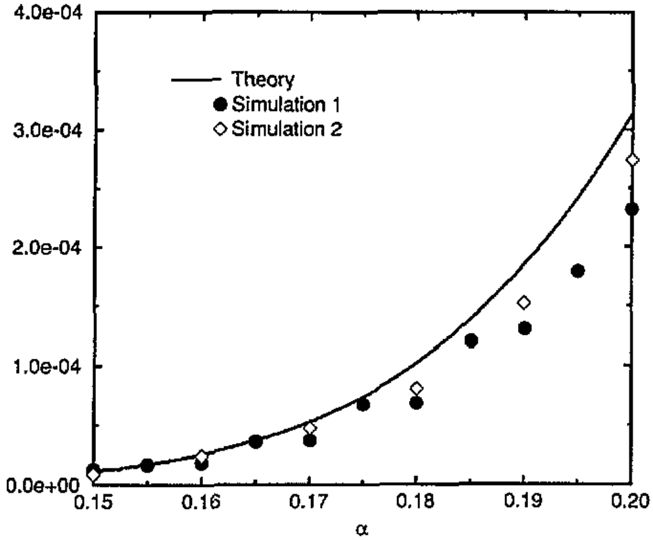

Figure 4. Effective diffusion constants are plotted as a function of a 'bare' diffusion constant. For comparison, two data sets obtained from numerical simulations are also plotted. Below $\alpha \approx 0.17$, the fitting is satisfactory.

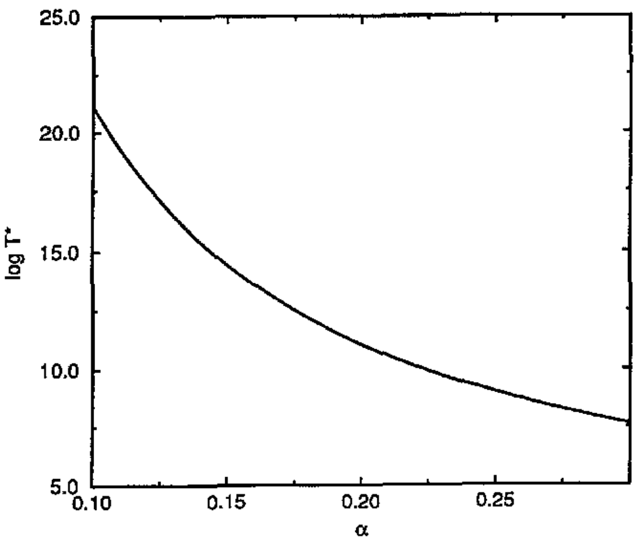

Figure 5. Logarithm of characteristic times T_α^* during which the particle is confined to the original minimum are plotted as a function of a diffusion constant.

holds for a given value of α; $\langle q^2 \rangle > 4\pi^2$ implies that the particle begins to diffuse to the next minimum. For $T < T_\alpha^*$, the particle motion is confined to the original minimum. In figure 5, we show the plot of this characteristic time T_α^*. Since the values of $\langle q^2 \rangle$ used here is an upper bound, that for T_α^* is a lower bound. For $\alpha \leqslant 0.17$, this is a very good lower bound. For $\alpha < 0.2$, the characteristic time is larger than 10^{10}.

In conclusion, we have calculated the probability distribution of Brownian motion in a cosine potential for a weak noise using the 'instanton' treatment of quantum field theory under some assumptions. The mean-squared deviation and the effective diffusion constant have also been calculated. Comparison of these results with numerical simulations are satisfactory where the 'instanton' treatment is valid, and the calculated values of the effective diffusion constants give an upper bound even in the region where the treatment is invalid. The characteristic time during which a particle is effectively confined to a particular minimum has been defined for a given value of the diffusion constant. This characteristic time becomes very long when the diffusion constant becomes small.

Acknowledgments

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Appendix A. The action of a single instanton

The instanton path satisfies the Euler–Lagrange equation

$$\ddot{q} = \sin q \cos q + \alpha \sin q \,.$$

Multiplying this by $\dot{q}$, we have

$$(\dot{q})^2 = \tfrac{1}{2}\,(1 - \cos 2q) + 2\alpha\,(1 - \cos q) \ .$$

Thus, the time derivative of the instanton path satisfies the equation,

$$\dot{q} = \sqrt{\sin^2 q + 4\alpha \sin^2 \frac{q}{2}} \,. \tag{A1}$$

The action of a single instanton is calculated as follows:

$$\begin{aligned} S_0 &= \int_{-T/2}^{T/2} \mathrm{d}\tau \tfrac{1}{2}\big[\,(\dot{q} + \sin q)^2 + 2\alpha\,(1 - \cos q)\,\big] \\ &\cong \int_{-\infty}^{\infty} \mathrm{d}\tau \tfrac{1}{2}\big[\,(\dot{q} + \sin q)^2 + 2\alpha\,(1 - \cos q)\,\big] \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \tfrac{1}{2}\left(\dot{q}^2 + \sin^2 q + 4\alpha \sin^2 \frac{q}{2}\right) + \int_{-\infty}^{\infty} \mathrm{d}\tau\, \dot{q} \sin q \,. \end{aligned}$$

The second term vanishes, and, using (A1), we have

$$\begin{aligned} S_0 &\cong \int_{-\infty}^{\infty} \mathrm{d}\tau\, (\dot{q})^2 = \int_0^{2\pi} \mathrm{d}q\, \dot{q} \\ &= \int_0^{2\pi} \mathrm{d}q \sqrt{\sin^2 q + 4\alpha \sin^2 \frac{q}{2}} \\ &= 4\left(\sqrt{1+\alpha} + \alpha \log \frac{1 + \sqrt{1+\alpha}}{\sqrt{\alpha}}\right). \end{aligned}$$

Appendix B. The fluctuation around the one-instanton path

In this appendix, we show the detailed description of the calculation of the factor K in section 2.

An instanton is a classical particle which moves in a potential

$$V(q) = \tfrac{1}{4}\cos 2q + \alpha \cos q\,.$$

In order to include fluctuations around a one-instanton path, we write an arbitrary path as an instanton plus fluctuation around it,

$$q(t) = \bar{q}(t) + \delta q(t)$$

where we denote an instanton as $\bar{q}(t)$. The contribution from this one-instanton path to $P_{2n\pi}$ is

$$\begin{aligned}
\mathcal{N}\int \mathcal{D}q \exp\left(-\frac{1}{2\alpha}S\left[q(t)\right]\right)
&= \mathcal{N}\mathrm{e}^{-S_0/2\alpha}\int \mathcal{D}[\delta q]\exp\left[-\frac{1}{2\alpha}\int_{-\infty}^{\infty}\mathrm{d}t\,\tfrac{1}{2}\delta q\left(-\partial_t^2 + V''(\bar{q})\right)\delta q\right] \\
&= \mathcal{N}\mathrm{e}^{-S_0/2\alpha}\left[\det\left(-\partial_t^2 + V''(\bar{q})\right)\right]^{-1/2} \qquad \text{(B1)}
\end{aligned}$$

where $V''(q)$ is the second derivative of $V(q)$, and $\det\left(-\partial_t^2 + V''(\bar{q})\right)$ is the determinant of the operator $\left(-\partial_t^2 + V''(\bar{q})\right)$. The operator $\left(-\partial_t^2 + V''(\bar{q})\right)$ has, however, the zero-modes; we can verify that $\dot{\bar{q}}/\sqrt{S_0}$ is indeed the solution of the zero-mode eigenvalue equation

$$\left(-\partial_t^2 + V''(\bar{q})\right)q_0(t) = 0$$

with the normalization condition of the solution

$$\int_{-\infty}^{\infty}\mathrm{d}t[q_0(t)]^2 = 1\,.$$

Thus, (B1) diverges at first sight.

This divergence is fictitious. It is known that the integration of the amplitude of the zero-mode fluctuation is identical to the translational freedom of the 'jump' time of an instanton within the time interval $(-T/2,\, T/2)$, and that the factor $\sqrt{S_0/4\pi\alpha}T$ takes care of this integration [4].

Thus, (B1) becomes

$$\mathcal{N}\mathrm{e}^{-S_0/2\alpha}\sqrt{\frac{S_0}{4\pi\alpha}}T\left[\det'\left(-\partial_t^2 + V''(\bar{q})\right)\right]^{-1/2} \qquad \text{(B2)}$$

where det′ means the determinant with the zero eigenvalues excluded.

On the other hand, this is equal to

$$\frac{(1+\alpha)^{1/4}}{\sqrt{4\pi\alpha}}\mathrm{e}^{-T(1+\alpha)/2}KT\mathrm{e}^{-S_0/2\alpha}\,. \qquad \text{(B3)}$$

It can be proved that

$$\frac{(1+\alpha)^{1/4}}{\sqrt{4\pi\alpha}}\mathrm{e}^{-T(1+\alpha)/2} = \mathcal{N}\left[\det\left(-\partial_t^2 + 1 + \alpha\right)\right]^{-1/2}.$$

After equating (B2) with (B3), we have

$$\begin{aligned}
K &= \sqrt{\frac{S_0}{4\pi\alpha}}\left[\frac{\det\left(-\partial_t^2 + 1 + \alpha\right)}{\det'\left(-\partial_t^2 + V''(\bar{q})\right)}\right]^{1/2} \\
&= \sqrt{\frac{S_0}{4\pi\alpha}} \times \tilde{K}\,. \qquad \text{(B4)}
\end{aligned}$$

Now, we proceed with the calculation of $\tilde{K}$. We calculate this quantity with the aid of the Fredholm determinant [6].

The Fredholm determinant is defined as

$$\Delta(E) \equiv \frac{\det\left(\hat{H} - E\right)}{\det\left(\hat{H}_0 - E\right)}$$

with respect to two operators $\hat{H}$ and $\hat{H}_0$. This is a function of a real parameter E. In our problem,

$$\hat{H} = -\partial_t^2 + V''(\bar{q})$$

and

$$\hat{H}_0 = -\partial_t^2 + 1 + \alpha\,.$$

It should be noted that

$$V''(\bar{q}) \to 1 + \alpha \qquad t \to \pm\infty\,.$$

(We write $\tilde{\beta}^2 = 1 + \alpha$ in the following.)

Using this Fredholm determinant, we can evaluate $\tilde{K}$ as follows:

$$\begin{aligned} \tilde{K} &= \left[\frac{\det \hat{H}_0}{\det' \hat{H}}\right]^{1/2} = \lim_{E\to 0}\left[\frac{\prod_n' (E_n - E)}{\prod_n (E_{0n} - E)}\right]^{-1/2} \\ &= \lim_{E\to 0}\left(-\frac{\Delta(E)}{E}\right)^{-1/2} = \left(-\Delta'(0)\right)^{-1/2} \end{aligned} \tag{B5}$$

where E_n and E_{0n} are the eigenvalues of $\hat{H}$ and $\hat{H}_0$, respectively; $\prod'$ means the product with the zero eigenvalues is excluded.

For the evaluation of $\Delta'(0)$, we borrow a technique from 1D scattering theory. Let us consider the scattering problem represented by the Schrödinger equation

$$\left[-\partial_t^2 + V''(\bar{q})\right]\psi = E\psi \tag{B6}$$

where $E > \tilde{\beta}^2$. The solutions are parametrized by E. There is a two-fold degeneracy of the solutions for each value of E, reflecting the fact that the wave can approach from either direction. These solutions, denoted by $f_\pm(t, E)$, have the following asymptotic forms:

$$\begin{aligned} &f_\pm(t, E) \to \mathrm{e}^{\pm ikt} && t \to \pm\infty \\ &f_\pm(t, E) \to \mathrm{e}^{\mp ikt} A_\pm(E) + \mathrm{e}^{\pm ikt} F_\pm(E) && t \to \mp\infty \end{aligned} \tag{B7}$$

where $k^2 = E - \tilde{\beta}^2$. The reason that we take these asymptotic forms is because it is known that

$$F_+(E) = F_-(E) = \Delta(E)\,.$$

The Wronskian is defined as

$$W\left[f_+(t, E), f_-(t, E')\right] \equiv f_+(t, E)\partial_t f_-(t, E') - \partial_t f_+(t, E) f_-(t, E')\,.$$

Taking the time derivative of the Wronskian and using the fact that $f_\pm(t, E)$ are the solutions of (B6), we have

$$\partial_t W\left[f_+(t, E), f_-(t, E')\right] = (E - E') f_+(t, E) f_-(t, E')\,.$$

We are now interested in the case that $E, E' \approx 0$, because we want to calculate $\Delta'(0)$. We know that the zero-mode solution is proportional to $\dot{\bar{q}}$. The asymptotic form of $\dot{\bar{q}}$ is calculated from (14),

$$\dot{\bar{q}} \to 4\frac{1+\alpha}{\sqrt{\alpha}}\mathrm{e}^{-\tilde{\beta}t} = A\mathrm{e}^{-\tilde{\beta}t} \qquad t \to \pm\infty .$$

So that

$$f_\pm(t,0) = \frac{\dot{\bar{q}}}{A} .$$

Thus,

$$\partial_E \partial_t W \to f_+(t,0) f_-(t,0) = \frac{(\dot{\bar{q}})^2}{A^2} \qquad E, E' \to 0 .$$

After integrating with respect to t from $-\infty$ to ∞, we have

$$\int_{-\infty}^{\infty} \mathrm{d}t\, \partial_E \partial_t W \to \frac{1}{A^2}\int_{-\infty}^{\infty} \mathrm{d}t\, (\dot{\bar{q}})^2 = \frac{S_0}{A^2} \qquad E, E' \to 0 . \tag{B8}$$

On the other hand, when $E \approx 0$, the asymtotic forms (B7) become

$$\begin{aligned} f_\pm(t,E) &\to \mathrm{e}^{-\tilde{\beta}|t|} && t \to \pm\infty \\ f_\pm(t,E) &\to \mathrm{e}^{-\tilde{\beta}|t|} A_\pm(E) + \mathrm{e}^{\tilde{\beta}|t|}\Delta(E) && t \to \mp\infty . \end{aligned} \tag{B9}$$

Using this, the leading terms of the Wronskians are

$W\left[f_+(t,E), f_-(t,E')\right] \cong 2\tilde{\beta}\Delta(E')$ for $E \approx E' \approx 0$ and $t \to \infty$

and

$W\left[f_+(t,E), f_-(t,E')\right] \cong 2\tilde{\beta}\Delta(E)$ for $E \approx E' \approx 0$ and $t \to -\infty$.

Hence

$$\int_{-\infty}^{\infty} \mathrm{d}t\, \partial_t W = 2\tilde{\beta}(\Delta(E') - \Delta(E)) .$$

Thus

$$\partial_E \int_{-\infty}^{\infty} \mathrm{d}t\, \partial_t W = -2\tilde{\beta}\Delta'(E) \to -2\tilde{\beta}\Delta'(0) \qquad E, E' \to 0 . \tag{B10}$$

Equating (B8) and (B10), we have

$$-2\tilde{\beta}\Delta'(0) = \frac{S_0}{A^2} .$$

So,

$$-\Delta'(0) = \frac{S_0}{2\tilde{\beta}A^2} .$$

From (B5),

$$\begin{aligned} \tilde{K} &= \sqrt{\frac{2\tilde{\beta}}{S_0}}A \\ &= 4\sqrt{\frac{2}{S_0}}\frac{(1+\alpha)^{5/4}}{\sqrt{\alpha}} . \end{aligned}$$

This completes the calculation of K. From (B4),

$$K = \sqrt{\frac{S_0}{4\pi\alpha}}\tilde{K} = \frac{4}{\sqrt{2\pi}}\frac{(1+\alpha)^{5/4}}{\alpha} .$$

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