Изв. вузов «ПНД», т.11, № 2, 2003 УДК 531.19:519.217

EXACT CALCULATION OF EFFECTIVE DIFFUSION CONSTANT IN FLUCTUATING PERIODIC POTENTIALS

A.A. Dubkov

Exact formula for diffusion coefficient of Brownian particle moving in modulated by white noise periodic field is obtained. As it is shown the acceleration of diffusion in comparison with a free diffusion case takes place for an arbitrary potential profile. Calculations of effective diffusion constant for different periodic potentials are performed.

Introduction

The problem of diffusion in periodic potential is related to a rich variety of physical situations such as diffusion of atoms in crystals, «ad-atom» moving near a solid surface, synchronization of oscillations, fluctuations of a Josephson supercurrent and so on. During the 1970's, an exact expressions for diffusion constant was independently obtained in the overdamped limit by various methods for an arbitrary periodic potential [1] and for sinusoidal potential [2]. Recently the mean velocity and effective diffusion coefficient of Brownian particle moving in a tilted periodic potential have been found in [3].

At the same time, the case of time-varying periodic potential is also of interest to practice. So, diffusion in fast fluctuating periodic field was the subject of investigation in [4]. Author derived the exact result for effective diffusion constant in the serrated potential. Present paper is generalization of results [4] on the case of arbitrary potential profiles.

Derivation of effective diffusion coefficient

We consider an overdamped Brownian particle in fluctuating periodic potential $U(x)$ whose dynamics is governed by the Langevin equation

$$dx/dt = -\zeta(t)dU(x)/dx + \xi(t) \tag{1}$$

where $x(t)$ is the displacement in time t, $\xi(t)$ and $\zeta(t)$ are statistically independent Gaussian white noises with zero means and intensities D and D_ζ respectively. Further we assume that potential $U(x)$ is even function with period L and place the origin in one of potential minima.

Following [1], [2] we determine the diffusion constant as the limit

$$D_\infty = \lim_{t\to\infty}\langle x^2(t)\rangle/t = \lim_{t\to\infty} d\langle x^2(t)\rangle/dt \qquad (2)$$

because in considering case $\langle x(t)\rangle=0$. It is easy matter to write from Eq. (1) the Fokker-Planck equation for probability density $W(x,t)$[1]

$$\partial W/\partial t = (D_\zeta/2)(\partial U'(x)/\partial x)(\partial(U'(x)W)/\partial x) + (D/2)\partial^2 W/\partial x^2 . \qquad (3)$$

Since we interest an asymptotic behaviour of mean square coordinate of Brownian particles the initial condition for Eq. (3) may be chosen arbitrarily. With this possibility we place all Brownian particles in the origin at t=0: $W(x,0)=\delta(x)$. In view of evenness of potential $U(x)$ the diffusion will go symmetrically in both directions of x-axis and the probability flow at the point x=0 will be equal to zero. This means that for calculation of D_∞ we can place the reflecting boundary in the origin and consider a diffusion in a positive direction of x-axis only.

Let introduce into consideration the Laplace transform of probability density

$$Y(x,s) = \int_0^\infty W(x,t)\exp(-st)dt.$$

As a result Eq. (3) becomes the second-order ordinary differential equation for function $Y(x,s)$

$$(D/2)(d^2Y/dx^2) + (D_\zeta/2)(dU'(x)/dx)(d(U'(x)Y)/dx) - sY = 0 \quad (x>0). \qquad (4)$$

In addition to Eq. (4) we should write the normalization condition for probability density

$$\int_0^\infty Y(x,s)dx = 1/s. \qquad (5)$$

Upon Floquet's theorem [5] linear homogeneous differential Eq. (4) with periodic coefficients has the next finite solution in the area x>0

$$Y(x,s) = \exp(-\mu(s)x)\Phi(x,s) \qquad (6)$$

where $\Phi(x,s)$ is periodic function with the same period L and $\mu(s)$ is the characteristic exponent of solution. The positive exponent $\mu(s)\to 0$ when $s\to 0$ by virtue of the fact that Eq. (4) has periodic solution at s=0.

Based on the limiting theorems of Laplace transform we obtain from Eq. (2)

$$D_\infty = \lim_{s\to 0} s^2\overline{x_s^2} \qquad (7)$$

where

$$\overline{x_s^2} = \int_0^\infty x^2 Y(x,s)dx = \partial^2/\partial\mu^2 \int_0^\infty \exp(-\mu x)\Phi(x,s)dx. \qquad (8)$$

Because the value $\overline{x_s^2}$ enters into the limit (7) it is sufficient to find an approximate expression for the integral in Eq. (8) at $s\to 0$ (i.e. $\mu\to 0$). Taking into account the periodicity of function $\Phi(x,s)$ in Eq. (6) and the normalization condition (5) we have

$$1/s = \Sigma_{n=0}^{\infty}\int_{nL}^{(n+1)L} \exp(-\mu x)\Phi(x,s)dx =$$

$$= \int_0^L \exp(-\mu x)\Phi(x,s)dx\, \Sigma_{n=0}^{\infty}\exp(-\mu nL) \simeq 1/(\mu L)\int_0^L \exp(-\mu x)\Phi(x,s)dx.$$

Thus,

---

[1] We interpret Eq. (1) in symmetrized Stratonovich form in order to obtain parametric effects.

$$\overline{x_s^2} \simeq 2/(\mu^3 L)\int_0^L \exp(-\mu x)\Phi(x,s)dx \simeq 2/(s\mu^2). \qquad (9)$$

Substitution of Eq. (9) into Eq. (7) leads to a new expression for diffusion coefficient in the form of limit

$$D_\infty = 2\lim_{s\to 0} s/(\mu^2(s)). \qquad (10)$$

As it is obvious from Eq. (10) the problem is reduced to calculation of the characteristic exponent $\mu(s)$ of Eq. (4). This calculation, as a rule, presents a certain difficulties associated with a zero condition for infinite determinant [5]. But in this situation we can derive the exponent $\mu(s)$ directly from Eq. (4) based on small value of μ.

First of all, let us replace the variable $Y(x,s)$ by $Z(x,s)=[D+D_\xi(U'(x))^2]^{1/2}Y(x,s)$ and rewrite Eq. (4) in the form

$$(D/2)d^2Z/dx^2 + (D_\xi/2)U'(x)dU'(x)/dx\ dZ/dx - sZ = 0. \qquad (11)$$

Since the multiplier $[D+D_\xi(U'(x))^2]^{1/2}$ is a periodic function the characteristic exponent of Eq. (11) coincides with $\mu(s)$. By above-mentioned Floquet's theorem the characteristic exponent of Eq. (11) for an even functions $U(x)$ can be found from the equation

$$\cosh\mu L = Z_1(L,s), \qquad (12)$$

where $Z_1(x,s)$ is the particular solution of Eq. (11) which satisfies the conditions

$$Z_1(0,s) = 1, \quad Z_1'(0,s) = 0. \qquad (13)$$

Using a small value s we can expand $Z_1(x,s)$ in power series

$$Z_1(x,s) = z_0(x) + sz_1(x) + \dots \qquad (14)$$

and obtain the next expressions after substitution Eq. (14) into Eq. (11) and equating the terms with the same powers of s

$$\begin{aligned}(D/2)d^2z_0/dx^2 + (D_\xi/2)U'(x)dU'(x)/dx\ dz_0/dx = 0,\\ (D/2)d^2z_1/dx^2 + (D_\xi/2)U'(x)dU'(x)/dx\ dz_1/dx = z_0.\end{aligned} \qquad (15)$$

The conditions for functions $z_0(x)$ and $z_1(x)$ can be found from Eqs (13), (14)

$$z_0(0) = 1, \quad z_0'(0) = 0, \quad z_1(0) = 0, \quad z_1'(0) = 0. \qquad (16)$$

The solution of the first Eq. (15) with conditions (16) is very simple: $z_0(x)=1$. Substituting the expansion (14) in Eq. (1) we find approximately the characteristic exponent $\mu^2(s)\simeq 2sz_1(L)/L^2$ and after substitution in Eq. (10) get the exact result

$$D_\infty = L^2/z_1(L) \qquad (17)$$

where the value $z_1(L)$ has dimension of time and must be calculated from the second Eq. (15)

$$(D/2)d^2z_1/dx^2 + (D_\xi/2)U'(x)dU'(x)/dx\ dz_1/dx = 1 \qquad (18)$$

with condition (16).

Rewriting Eqs (16)-(18) in terms of new variable $\tau(x)=z_1(L)-z_1(x)$ we obtain

$$D_\infty = L^2/\tau(0) \qquad (19)$$

where $\tau(x)$ satisfies well-known equation for the mean first-passage time

$$\tau''(x)D/2 + \tau'(x)(D_\xi/2)U'(x)dU'(x)/dx = -1 \quad (20)$$

with boundary conditions

$$\tau'(0) = 0, \quad \tau(L) = 0. \quad (21)$$

Thus, we arrive at the conclusion that the problem of calculating the diffusion coefficient D_∞ reduces to determining the mean first-passage time of an absorbing boundary $x=L$ for Brownian particles starting from the reflecting boundary at the point $x=0$. It should be noted that the equivalence of the definitions (2) and (19) was first demonstrated in paper [6] for fixed periodic field. By analogy with the expression for free diffusion ($U(x)=0$) the diffusion coefficient (19) was called in [6] as effective constant.

Solving Eq. (20) with conditions (21) we obtain the exact formula finally for diffusion coefficient of Brownian particle in fast fluctuating periodic potential $U(x)$

$$D_\infty = D[1/L \int_0^L (1+D_\xi(U'(x))^2/D)^{-1/2}dx]^{-2}. \quad (22)$$

As it is obvious from Eq. (22) $D_\infty < D$ for arbitrary potential profile $U(x)$, i.e. diffusion of Brownian particles accelerates in comparison with the case $U(x) = 0$. This result fully confirms the assumption previously proposed in [4]. We emphasize that the value of diffusion constant depends not on a height of potential barriers as for fixed potential [1,2], but on its gradient $U'(x)$.

It is easily to explain the phenomenon of diffusion acceleration directly from Eq. (19) as in [4]. The point is that potential barriers change a place through a random modulation and Brownian particles move from point $x=0$ to point $x=L$ more rapidly in comparison with free diffusion case (in the average particles move downhill for the most part of the distance).

Examples

Let us consider some particular shapes of potential $U(x)$. For the serrated profile $U(x)=2E|x|/L$ at $|x|\leq L/2$ we instantly arrive at Malakhov's exact result [4]

$$D_\infty = D + D_\xi 4E^2/L^2. \quad (23)$$

On the other hand, we obtain for sinusoidal potential $U(x)=E\sin^2(\pi x/L)$ from Eq. (22)

$$D_\infty = \pi^2 D(1+\gamma^2)/[4\mathbf{K}^2(\gamma/(1+\gamma^2)^{1/2})], \quad \gamma = \pi E/L(D_\xi/D)^{1/2}, \quad (24)$$

where $\mathbf{K}(k)$ is complete elliptic integral of the first kind ($0<k<1$). We derive from Eq. (24) at small strength D_ξ of modulating white noise ($\gamma<<1$)

$$D \simeq D + D_\xi \pi^2 E^2/(2L^2).$$

This formula coincides with approximate result [4] obtained on the assumption of Gaussian probability density $W(x,t)$ although the real probability density is multimodal. In opposite case $\gamma>>1$ using the asymptotic formula for elliptic integral [7]

$$\mathbf{K}(k) \simeq \ln(4/(1-k^2)^{1/2}) \qquad (k\to 1),$$

we find from Eq. (24)

$$D_\infty \simeq D(\pi\gamma)^2/(4\ln^2\gamma) \sim D_\xi/(\ln^2 D_\xi). \quad (25)$$

According to Eq. (25) the effective diffusion coefficient increases with intensity D_ξ of modulating noise but more slow than linear law (23).

At last, for periodic potential profile representing by parabolic pieces

$$U(x) = \begin{cases} 8E(x/L)^2, & |x| \le L/4 \\ E[1-8(x/L - {}^1/_2)^2], & L/4 \le x \le {}^3/_4 L \end{cases}$$

it is not difficult to derive from the exact formula (22) the following result

$$D_\infty = Dm^2/\ln^2(m+(1+m^2)^{1/2}), \qquad m = 4E/L(D_\zeta/D)^{1/2}.$$

As it is seen at comparatively small intensity D_ζ (m<<1)

$$D_\infty \simeq D + D_\zeta 16E^2/(3L^2)$$

that is differed a little from formula for sinusoidal potential. Moreover, the dependence of effective diffusion coefficient on large D_ζ is similar to the law (25) for sinusoidal potential profile.

Conclusion

We studied the diffusion of an overdamped Brownian particle in a fast fluctuating periodic potential and calculated the effective diffusion coefficient. The exact formula (22) obtained points to a diffusion acceleration in comparison with a free diffusion case for any potential profiles. We offered an explanation of the above-mentioned phenomenon and considered the different shapes of potentials. Our results may be of interest in modern diffusive technologies.

This work has been supported by Russian Foundation for Basic Research (projects 00-15-96620, 02-02-17517), INTAS (grant 2001-0450), and Scientific Program «Universities of Russia» (project UR.01.01.008).

References

1. *Festa R., d'Agliano E.G.* Diffusion coefficient for a Brownian particle in a periodic field of force. I. Large friction limit // Physica A. 1978. Vol. 90. P. 229.

2. *Medvedev S.Yu., Saichev A.I* . Exact calculation of phase diffusion constant for synchronized generator // Radiotekhika i Electronika. 1979. Vol. 24, № 10. P. 2058.

3. *Lindner B., Kostur M. and Schimansky-Geier L.* Optimal diffusive transport in a tilted periodic potential // Fluct. and Noise Lett. 2001. Vol. 1, № 1. P. R25.

4. *Malakhov A.N* . Acceleration of Brownian particle diffusion parallel to a fast random field with a short spatial period // Technical Physics Letters. 1998. Vol. 24, №. 11. P. 833.

5. *Zwillinger D*. Handbook of Differential Equations. 3rd ed. Boston, MA. Academic Press, 1997.

6. *Weaver D.L.* Effective diffusion coefficient of a Brownian particle in a periodic potential // Physica A. 1979. Vol. 98. P. 359.

7. Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables / Eds *M. Abramowitz and I.A. Stegun* . Dover Publications, Inc., New York, 1972.

Нижегородский государственный университет

Поступила в редакцию 19.11.02
после доработки 14.02.03

ТОЧНЫЙ РАСЧЕТ ЭФФЕКТИВНОЙ ПОСТОЯННОЙ ДИФФУЗИИ ВО ФЛУКТУИРУЮЩИХ ПЕРИОДИЧЕСКИХ ПОТЕНЦИАЛАХ

А.А. Дубков

Получена точная формула для коэффициента диффузии броуновской частицы, движущейся в модулируемом белым шумом периодическом поле. Показано, что для любого потенциального профиля наблюдается ускорение диффузии по сравнению со случаем свободной диффузии. Выполнены расчеты эффективной диффузионной постоянной для различных периодических потенциалов.

Дубков Александр Александрович - родился в Горьком (1949), окончил радиофизический факультет Горьковского, ныне Нижегородского, государственного университета (1972). После окончания работает в должности доцента ННГУ. Защитил диссертацию на соискание ученой степени кандидата физико-математических наук в ННГУ (1981) в области статистической радиофизики. В настоящее время является докторантом ННГУ и заканчивает работу над докторской диссертацией. Опубликовал 50 научных статей в области статистической физики и радиофизики, теории случайных процессов, динамического хаоса и турбулентности.

E-mail: dubkov@rf.unn.ru