

Langevin dynamics with dichotomous noise; direct simulation and applications

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Abstract

We consider the motion of a Brownian particle moving in a potential field and driven by dichotomous noise with exponential correlation. Traditionally, the analytic as well as the numerical treatments of the problem, in general, rely on Fokker-Planck description. We present a method for direct numerical simulation of dichotomous noise to solve the Langevin equation. The method is applied to calculate nonequilibrium fluctuation induced current in a symmetric periodic potential using asymmetric dichotomous noise and compared to Fokker-Planck-Master equation based algorithm for a range of parameter values. Our second application concerns the study of resonant activation over a fluctuating barrier.

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I. INTRODUCTION

Langevin equation^{1,2,3} is the key stochastic differential equation that encompasses a wide range of physical, chemical and biological sciences. Although originally envisaged as a descriptor of the motion of a Brownian particle in a fluid in thermal equilibrium, the equation is now the basic paradigm for almost any physically realizable stochastic process which takes into account of the motion of particle in phase space and at the same time acted upon by a noise force which may be internal or external depending on whether the fluctuation-dissipation relation is satisfied or not, respectively. Over the years various noise processes with arbitrary correlation time have been in use in a wide variety of problems, *e.g.*, in activated processes in kinetics^{4,5}, noise-induced transport processes^{6,7,8,9,10,11,12,13,14,15,16,17} in condensed matter and biological physics^{18,19,20,21} etc. Among others dichotomous or telegraphic noise^{22,23,24,25,26,27,28} plays the typical theoretician's paradigm of fluctuations in this context. While for linear potentials the Langevin equation with dichotomous noise is solvable analytically, arbitrary nonlinear potential poses serious problems. For example, it is very difficult, if not impossible, to treat a ratchet device with periodic potential and finite correlation time of noise. One therefore routinely takes resort to an equivalent Fokker-Planck approach and the algorithm based on this description. The notable point is that the approach bypasses the generation of dichotomous noise as such and a close survey of the recent literature suggests that a direct simulation of Langevin dynamics of a particle driven by dichotomous noise still remains to be addressed. Our object in this paper is thus twofold,

(i) We present a general numerical algorithm for generation of dichotomous noise with exponential correlation and numerically simulate the Langevin dynamics for the particle without taking resort to any Fokker-Planck or master equation description.

(ii) As two prototypical applications with additive and multiplicative noise processes we consider dichotomous noise-induced transport or current in a periodic potential in a ratchet device and resonant activation over a fluctuating barrier.

In implementing the scheme it is essential to take care of the fact that the numerical error should not bring any additional tilt to the potential or break of any inversion symmetry or detailed balance of the system. Second, the forcing terms must be unbiased so that after appropriate averaging over time, space and ensemble no directed transport should appear as an artifact. These considerations are particularly important for thermodynamic

consistency^{29,30,31,32,33,34} of the numerical scheme. Thus although the numerical simulation of Langevin dynamics with dichotomous noise is useful in a wide variety of other situations, our choice of application here is guided by these considerations.

The outline of the paper is as follows: In Sec.II we present our method of numerical solution of Langevin equation in presence of an internal noise and a dichotomous noise. Although the elements of the present numerical scheme are commonly used in Monte Carlo calculations, the implementation in generating dichotomous noise in the numerical solution of Langevin equation for realization of stochastic path and nonequilibrium fluctuation-induced transport and resonant activation are new in the current context. Sec.III is devoted to the numerical results on the noise induced current for a cosine potential. We compare the methods based on Langevin equation and Fokker-Planck equation¹³ for a range of parameters. Another application is the study of activated escape over a fluctuating barrier. The paper is concluded in Sec.IV.

II. NUMERICAL SIMULATION OF LANGEVIN DYNAMICS WITH DICHOTOMOUS NOISE

In order to motivate our numerical simulation method we consider the motion of an overdamped particle in a periodic potential, $V(x)$, simultaneously subjected to an internal thermal noise, $\xi(t)$, and an external dichotomous or telegraphic noise, $\eta(t)$. This is described by the Langevin equation of the following form

$$\dot{x}(t) = -V'(x) + \xi(t) + \eta(t) \quad (2.1)$$

The periodic potential $V(x)$ may be symmetric or asymmetric depending on the specificity of the situation. $\xi(t)$ is the thermal, Gaussian, white noise whose mean and variance are given by

$$\langle \xi(t) \rangle = 0 \quad (2.2)$$

$$\langle \xi(t)\xi(t') \rangle = 2k_B T \delta(t - t') \quad (2.3)$$

respectively, where k_B is the Boltzmann constant and T is the absolute temperature which is the measure of the strength of internal noise.

$\eta(t)$ is the dichotomous noise which can assume only two random values, say, a and b . We also require the random number sequence to satisfy:

$$\langle \eta(t) \rangle = 0 \quad (2.4)$$

$$\langle \eta(t)\eta(t') \rangle = \frac{Q}{\tau} \exp\left(-\frac{|t-t'|}{\tau}\right) \quad (2.5)$$

or in other words, the dichotomous noise must have a zero mean and be exponentially correlated. Q is the strength and τ is the correlation time of the dichotomous noise.

Our problem here is to find out the sample path $x(t)$ of the particle as a function of time and calculate the relevant quantities for nonequilibrium fluctuation-induced transport. More specifically, we calculate the average velocity of the particle under a steady state condition.

A. The algorithm

A simple approach for numerical simulation of Eq.(2.1) is to discretize time t and to use a predictor-corrector method in advancing the particle from $x(t_n)$ to $x(t_{n+1})$ as follows:

$$x_1(t_{n+1}) = x(t_n) - V'(x(t_n))\Delta t + \eta(t_n)\Delta t + (2k_B T \Delta t)^{1/2} W_n \quad (2.6)$$

$$x(t_{n+1}) = x(t_n) - \frac{1}{2} [V'(x(t_n)) + V'(x_1(t_{n+1}))] \Delta t + \eta(t_n)\Delta t + (2k_B T \Delta t)^{1/2} W_n \quad (2.7)$$

where the first step (2.6) implies the simplest Euler-type algorithm for the predictor, whereas the second step corresponds to the corrector. Δt is the time step and W_n is a Gaussian distributed random number with zero average and a variance of unity independently chosen at each step using a standard Box-Muller algorithm^{35,36,37,38}.

The next important step is the generation of dichotomous random number $\eta(t)$ with given properties (2.4, 2.5) such as, zero average and exponential correlation. To this end we proceed as follows:

B. Generation of dichotomous noise

We consider a random variable $\eta(t)$ which switches between two values a and b randomly in time. The rate of switching from a to b is μ_a and from b to a is μ_b . This two-step process

can be described by a probability loss-gain equation or master equation¹

$$\frac{d}{dt}P(a, t|x, t_0) = -\mu_a P(a, t|x, t_0) + \mu_b P(b, t|x, t_0) \quad (2.8)$$

$$\frac{d}{dt}P(b, t|x, t_0) = \mu_a P(a, t|x, t_0) - \mu_b P(b, t|x, t_0) \quad (2.9)$$

where $P(a, t|x, t_0)$ is the conditional probability that the variable $\eta(t)$ will assume the value a at some time t given that it was x at earlier time t_0 . $P(b, t|x, t_0)$ can be defined similarly.

The conservation of total probability demands

$$P(a, t|x, t_0) + P(b, t|x, t_0) = 1 \quad (2.10)$$

The initial condition for Eqs.(2.8) and (2.9) are given by:

$$P(x', t|x, t_0) = \delta_{x'x} \quad \text{at} \quad t = t_0 \quad (2.11)$$

Eq.(2.8) and (2.9) admit the following steady state solutions

$$P^s(a) = P(a, \infty|x, t_0) = \frac{\mu_b}{\mu_a + \mu_b} \quad (2.12)$$

$$P^s(b) = P(b, \infty|x, t_0) = \frac{\mu_a}{\mu_a + \mu_b}$$

The conditional probabilities $P(a, t|x, t_0)$ and $P(b, t|x, t_0)$ for time t can be obtained by solving the Eqs.(2.8) and (2.9) subject to the conditions (2.10), (2.11) and (2.12):

$$P(a, t|x, t_0) = \frac{\mu_b}{\mu_a + \mu_b} + \left(\frac{\mu_a}{\mu_a + \mu_b} \delta_{ax} - \frac{\mu_b}{\mu_a + \mu_b} \delta_{bx} \right) \exp [-(\mu_a + \mu_b)(t - t_0)] \quad (2.13)$$

$$P(b, t|x, t_0) = \frac{\mu_a}{\mu_a + \mu_b} - \left(\frac{\mu_a}{\mu_a + \mu_b} \delta_{ax} - \frac{\mu_b}{\mu_a + \mu_b} \delta_{bx} \right) \exp [-(\mu_a + \mu_b)(t - t_0)] \quad (2.14)$$

Eqs.(2.13) and (2.14) can be used to calculate the mean and variance of the dichotomous noise in the steady state as

$$\langle \eta(t) \rangle = \frac{a\mu_b - b\mu_a}{\mu_a + \mu_b} \quad (2.15)$$

$$\langle \eta(t)\eta(t') \rangle = \left(\frac{a\mu_b - b\mu_a}{\mu_a + \mu_b} \right)^2 + \frac{\mu_a\mu_b(a+b)^2}{(\mu_a + \mu_b)^2} \exp [-(\mu_a + \mu_b)(t - t')] \quad (2.16)$$

respectively. Eqs.(2.15) and (2.16) can be identified as dichotomous noise with given properties (2.4) and (2.5), respectively, provided

$$a\mu_b - b\mu_a = 0 \quad (2.17)$$

with the following identification

$$\tau = \frac{1}{\mu_a + \mu_b} \quad (2.18)$$

and

$$\frac{Q}{\tau} = \frac{\mu_a\mu_b(a+b)^2}{(\mu_a + \mu_b)^2} \quad (2.19)$$

Now Eq.(2.17) can be rearranged to show $\frac{\mu_a\mu_b(a+b)^2}{(\mu_a + \mu_b)^2} = ab$, which when used in (2.19) yields

$$Q = ab\tau \quad (2.20)$$

Furthermore, for convenience, we define an asymmetric parameter

$$\theta = |a| - |b| \quad (2.21)$$

For choosing a set of seven parameters a , b , μ_a , μ_b , Q , θ and τ it is pertinent to satisfy four relations (2.17), (2.18), (2.20) and (2.21). This implies that only three independent parameters are needed to specify the dichotomous noise $\eta(t)$ with zero mean and exponential correlation.

With these aforesaid preliminaries we are now in a position to generate realizations of a stochastic process for a dichotomous noise. This is done in the following way. Let the particle is located initially (t) at $x_n = a$. To determine whether the particle moves at time $t_1 = t + \Delta t$ to another site $x_{n+1} = b$ or remain at the same site $x_n = a$, we consider the following conditional probability as given by (2.13)

$$P(a, t_1 | a, t) = \frac{\mu_b}{\mu_a + \mu_b} + \frac{\mu_a}{\mu_a + \mu_b} \exp [-(\mu_a + \mu_b)\Delta t] \quad (2.22)$$

An uniformly distributed random number R between $[0, 1]$ is now generated by the computer. This number is then compared against the conditional probability (2.22). If $P(a, t_1|a, t) > R$, then we accept the value of the noise a , *i.e.*, $x_n = a$, else we accept the value b or $x_{n+1} = b$. If the value of noise is b at $t_1(= t + \Delta t)$ then we calculate the conditional probability of jumping to another site $x_{n+2} = a$ at $t_2(= t_1 + \Delta t)$ as

$$P(a, t_2|b, t_1) = \frac{\mu_b}{\mu_a + \mu_b} - \frac{\mu_b}{\mu_a + \mu_b} \exp[-(\mu_a + \mu_b)\Delta t] \quad (2.23)$$

On the other hand if the value of the noise is $x_{n+1} = a$ at $t_1(= t + \Delta t)$ we calculate the conditional probability $P(a, t_2|a, t_1)$ using (2.22). We then compare the probability $P(a, t_2|b, t_1)$ or $P(a, t_2|a, t_1)$ against another uniformly distributed random number R_1 between $[0, 1]$.

If $P(a, t_2|b, t_1)$ or $P(a, t_2|a, t_1) > R_1$ then the value of the noise at t_2 is $x_{n+2} = a$ else we accept $x_{n+2} = b$. By repeating the procedure we can generate a sequence of random numbers $\eta(t)$ switching between two values a and b .

It is important to note that the time interval between the two steps is always fixed and is equal to Δt which is much smaller than the correlation time (τ) of the noise ($\Delta t \ll \tau$).

Fig.1(a-b) shows two illustrative dichotomous noise profiles for several values of τ . A close look into the figures suggests that with increase of correlation time, residence time of a particular state increases on an average. In order to check the numerical accuracy of the method of generation of dichotomous noise $\eta(t)$ we first calculate its first moment $\langle \eta(t) \rangle$ satisfying the condition (2.17). The typical ensemble averaging is carried out over long time of 100×5000 time steps as well as over 1000 sample paths. The ensemble average $\langle \eta(t) \rangle$ is close to zero (less than $\sim 10^{-6}$ as determined numerically). In Fig.2 we calculate the normalized auto-correlation function $\frac{\langle \eta(t)\eta(t+t') \rangle}{\langle \eta(t)^2 \rangle}$ of the noise for $a = 6.0$, $b = -4.0$ for several given values of $\tau(0.5, 2.0$ and $5.0)$. The values of τ are compared to the correlation time obtained by the corresponding numerical fitting curves. The agreement is found to be satisfactory.

III. RESULTS: (A) APPLICATION TO NOISE INDUCED CURRENT

Having explored the method of generation of dichotomous noise we now proceed to solve the Langevin equation (2.1) or its discretized version (2.6) and (2.7). The typical sample paths for the particle for several values of noise strength Q are plotted in Fig.3. It is

apparent that while for symmetric noise ($\theta = 0$) the system does not feel any additional load, asymmetry in the dichotomous noise gives rise to an external tilt depending on the strength of noise. In what follows we note that this asymmetry induced tilt in the overall potential is particularly important for generation of current when the potential is symmetric. The important relevant quantity for our present study is the steady state average velocity which can be defined as

$$\langle v \rangle = \frac{1}{S} \sum_S \left(\frac{1}{\mathcal{T}} \frac{1}{N} \sum_N (x_N - x(0)) \right)_S \quad (3.1)$$

\mathcal{T} is the total time over which the displacements are averaged over for a particular sample path. The second averaging is over the number of sample paths, S . Ensemble averaging requires both \mathcal{T} and S to be sufficiently large.

We now consider a cosine potential, *i.e.*, $V(x) = \cos(x)$, a symmetric periodic potential with periodicity 2π . For the entire simulation work we have chosen the time step of integration $\Delta t = 0.01$, number of time step is typically of the order of 10^6 and the number of sample paths is around 1000. We have calculated the steady state average velocity as a function of correlation time τ of the dichotomous noise keeping the asymmetric parameter $\theta = 0$ and shown $\langle v \rangle$ vs. τ profile in Fig.4. As expected we observe that the average velocity is zero, since the potential as well as the external dichotomous noise are symmetric and there can not be any directed motion of the particle. Fig.4 thus serves as a thermodynamic consistency check for our numerical calculation.

In order to exhibit Brownian ratchet effect we now switch on the asymmetric parameter θ to a non-zero value so that $\theta \neq 0$. In Fig.5 we display the variation of current $\langle v \rangle$ as a function of correlation time τ for three different values of θ ($= -1, -2, -4$). As the magnitude of θ increases the peak value of the current increases significantly. When τ is small $\langle v \rangle$ tends to be vanishing. This is because in order to have a net directed motion it is required that the system must not relax to its equilibrium state instantaneously. On the other hand when τ is very large, the overdamped system gets too much time to reach its equilibrium so that on an average net flows in the left and right directions tend to equalize making a net drift current vanishingly small. The system behaves resonantly at some optimum value of correlation time τ of the dichotomous noise, for which the current is maximum.

In Fig.6(a-b) we exhibit the variation of current ($\langle v \rangle$) as a function of correlation time

τ of the dichotomous noise for two different values of asymmetry parameter θ given by solid lines using Langevin dynamics. The results are compared with those obtained using Fokker-Planck-Master equation¹³ with periodic boundary condition. In Fig.7(a-b) we make a comparison between $\langle v \rangle$ vs. Q profile (for two different values of τ) calculated by our Langevin method and the Fokker-Planck method. The agreement is found to be quite satisfactory and provides support to our simulation method based on Langevin dynamics.

(B) RESONANT ACTIVATION OVER A FLUCTUATING BARRIER

Our second application of the method concerns resonant activation - the well-known resonance effect^{39,40,41,42,43,44,45,46} which can be observed in the variation of mean first passage time as a function of flipping rate of fluctuation of the barrier height of a double well potential. For the present purpose we consider a situation where the fluctuation is dichotomic in nature, *i.e.*, the barrier height fluctuates between two values. The fluctuation in potential has been found to be important in several kinetic models^{43,44} for chemical reactions. We consider the potential of the form

$$V(x, t) = U(x) + \frac{1}{2}x^2\eta(t) \quad (3.2)$$

where $U(x)$ is a bistable potential ($-\frac{A}{2}x^2 + \frac{B}{4}x^4$, A and B being constants) with a barrier at metastable point $x = 0$ and two stable minima of the potential are at $x = \pm\sqrt{\frac{A}{B}}$. The fluctuations in the barrier height of the potential are due to dichotomous noise, $\eta(t) = \{a, b\}$, *i.e.*, the barrier height of the potential fluctuates between two states randomly. Under overdamped condition the reaction coordinate $x(t)$ is governed by the following Langevin equation

$$\gamma\dot{x} = Ax - Bx^3 + x\eta(t) + \xi(t) \quad (3.3)$$

$\xi(t)$ is the usual thermal internal noise as defined in Eq.(2.2) and Eq.(2.3) An important point of departure from the earlier equation (2.1) is the presence of a multiplicative noise (in the third term on the right hand side of Eq.(3.3)) which is Gaussian distributed and exponentially correlated. Since, the stochastic integrals are different in Statonovich and $\hat{\text{Ito}}$ definitions, the drift term corresponding to Langevin equation (3.3) is $Ax - Bx^3$ according to $\hat{\text{Ito}}$'s prescription, whereas Statonovich prescription provides a drift term of the form $Ax - Bx^3 + x$. The spurious drift component however is missing in $\hat{\text{Ito}}$'s definition. It is

therefore somewhat convenient to use $\hat{\text{Ito}}$'s scheme for direct simulation of Langevin equation. In what follows we adopt this scheme and use of the predictor-corrector steps as (with $\gamma = 1.0$);

$$x_1(t_{n+1}) = x(t_n) + [Ax(t_n) - Bx^3(t_n) + x(t_n)\eta(t_n)]\Delta t + (2k_B T \Delta t)^{1/2} W_n \quad (3.4)$$

$$x(t_{n+1}) = x(t_n) + \frac{1}{2}[\{Ax(t_n) - Bx^3(t_n) + x(t_n)\eta(t_n)\} + \{Ax_1(t_n) - Bx_1^3(t_n) + x_1(t_n)\eta(t_n)\}]\Delta t + (2k_B T \Delta t)^{1/2} W_n \quad (3.5)$$

where the averages and variances of the white and dichotomous noises are as given earlier in the context of Eq.(2.1)

To analyze the essential features of the activated escape following stochastic dynamics over a fluctuating potential barrier we numerically simulate the Langevin equation (3.4-3.5) using the method for dichotomous noise generation as developed in the preceding section with a very small time step ($\Delta t = 0.01$). In our simulation we follow the dynamics of the particle starting from the potential minimum at $x = -\sqrt{\frac{A}{B}}$ of the left well till it arrives at the barrier top at $x = 0$ where the particle is removed. The first passage time⁴⁷ being a statistical quantity due to random nature of the dynamics we calculate the statistical average of the first passage time over 2000 trajectories. We chose the parameters of the potential as $A = 0.5$ and $B = 0.1$ for the entire set of calculation. We present our simulation results in Fig.8 and Fig.9 for several values of temperatures and variance ($\frac{Q}{\tau}$) of dichotomous noise. From both the figures it is clear that the mean first passage time ($\langle T \rangle$) passes through a minimum as one increases the correlation time (τ) of dichotomic barrier fluctuation. It is apparent that the mean first passage time responds resonantly with the correlated fluctuations of the barrier height. As one increases the strength of the internal noise of heat bath the escape rate increases (or the mean first passage time decreases) and the resonance behavior is manifested at the very high flipping rate as evident from Fig.8. When the flipping rate of the barrier height is very high ($\frac{1}{\tau} \rightarrow 0$) the system effectively feels an average barrier height so the mean first passage time is independent of the flipping rate. This is evident from the inset of Fig.8. Fig.8 and Fig.9 show that the mean first passage time becomes almost independent of the correlation time in the limit of high correlation time or slow flipping rate.

IV. CONCLUSION

We have presented an algorithm for numerical simulation for generating dichotomous noise and solution of the Langevin equation. As immediate applications of the method we have calculated nonequilibrium fluctuation induced current due to asymmetric, exponentially correlated dichotomous noise in a symmetric periodic potential over a wide range of parameter values and resonant activation rate of barrier crossing in a double well potential. The method is compared to the Fokker-Planck equation based numerical technique for solving stochastic dynamics on a discrete lattice simulated by a Master equation and is found to be complementary and well-suited for calculation of ratchet effect. We emphasize that while the overwhelming majority of the treatment of various phenomena including barrier crossing dynamics, resonant activation, stochastic resonance using dichotomous noise rely heavily on Fokker-Planck-Master equation approach we anticipate that the present method of solution of Langevin dynamics by direct simulation of dichotomous noise will be useful for various purposes in these issues. The simulation method can be easily extended to other noise processes involving, for example, three state jump process and for a wide range of correlation time and potentials without much difficulty.

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Figure Captions

Fig.1: Generation of dichotomous noise profile for $a = 6$, $b = -4$ (a) $\tau = 0.05$ and (b) $\tau = 0.4$.

Fig.2: Plots of normalized correlation function vs. t' for $a = 6.0$, $b = -4.0$, for three different noise profiles with given correlation times $\tau = 0.5, 2.0$ and 5.0 . Bold circles corresponds to fitted curves.

Fig.3: Plot of sample paths of the particle against time for different dichotomous noise strength (Q) and asymmetry parameter (θ) with $D = 0.2$ and $\tau = 1.0$.

Fig.4: Plot of average velocity $\langle v \rangle$ with correlation time τ of dichotomous noise for asymmetry parameter $\theta = 0$, $D = 0.02$ and $Q = 1.0$.

Fig.5: Plot of $\langle v \rangle$ vs. τ with different values of θ for constant white noise strength $D = 0.02$ for constant dichotomous noise strength $Q = 3.0$.

Fig.6: (a) Average velocity ($\langle v \rangle$) vs. dichotomous noise correlation time (τ) profile is compared with Fokker-Planck-Master equation method (solid circle) for $\theta = -2.0$, $Q = 3.0$ and $D = 0.02$. Inset: Same plot but on a shorter time scale. (b) Same as in Fig.6(a) but for $\theta = -4.0$.

Fig.7: (a) Average velocity ($\langle v \rangle$) vs. dichotomous noise strength (Q) profile is compared with Fokker-Planck-Master equation method (solid circle) for $\tau = 0.5$, $\theta = -2.0$ and $D = 0.02$. (b) Same as in Fig.7(a) but for $\tau = 5.0$.

Fig.8: Mean first passage time ($\langle T \rangle$) vs. correlation time of dichotomous noise τ for $D = 0.1$ (box); $D = 1.5$ (circle) and $D = 3.0$ (triangle). (The inset: mean first passage time ($\langle T \rangle$) vs. correlation time of dichotomous noise τ on a log scale for $D = 0.1$) for $a = 2.0$ and $b = 1.0$.

Fig.9: Mean first passage time ($\langle T \rangle$) vs. correlation time of dichotomous noise τ for several values of variances of dichotomous noise [$a = 3.0$, $b = 2.0$ (triangle); $a = 2.5$, $b = 1.5$ (circle) and $a = 2.0$, $b = 1.0$ (square)] for $D = 0.1$.

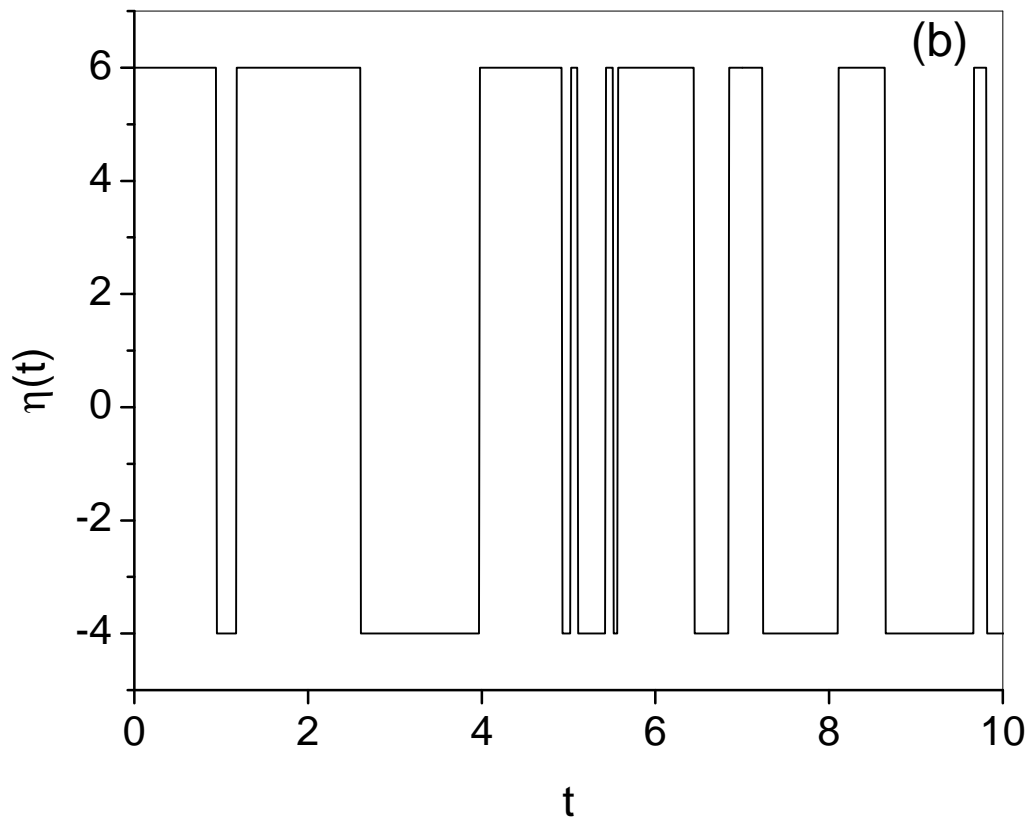
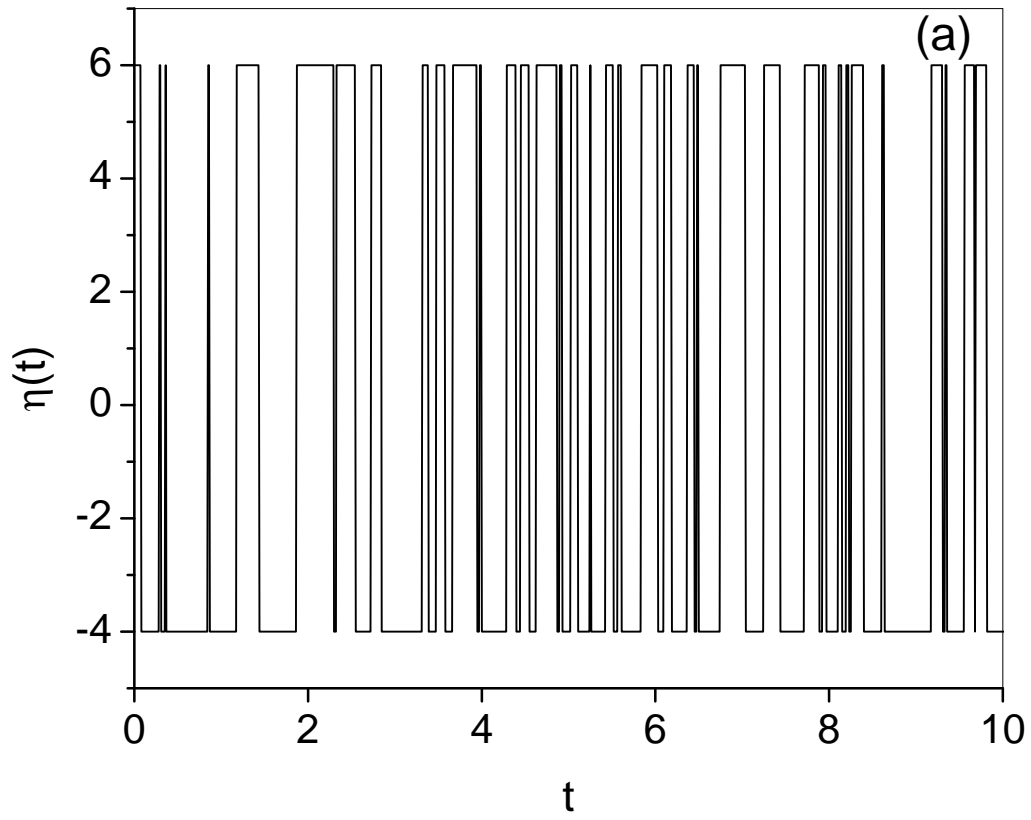


Fig.1

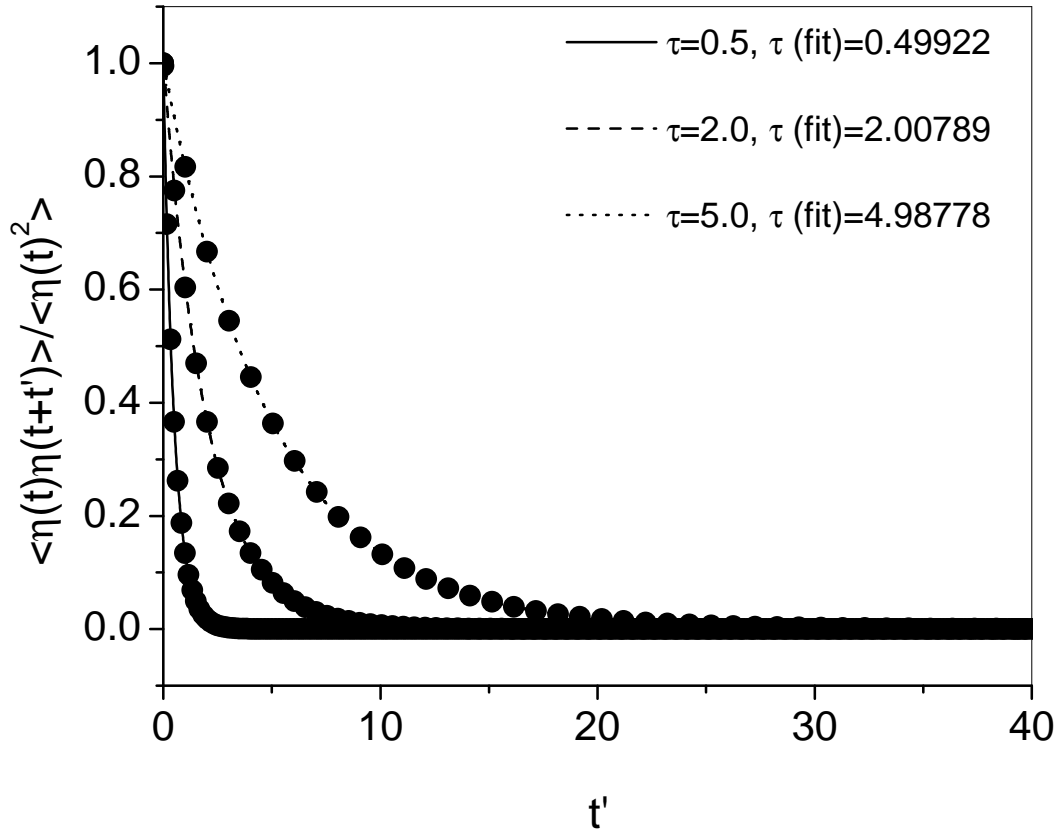


Fig.2

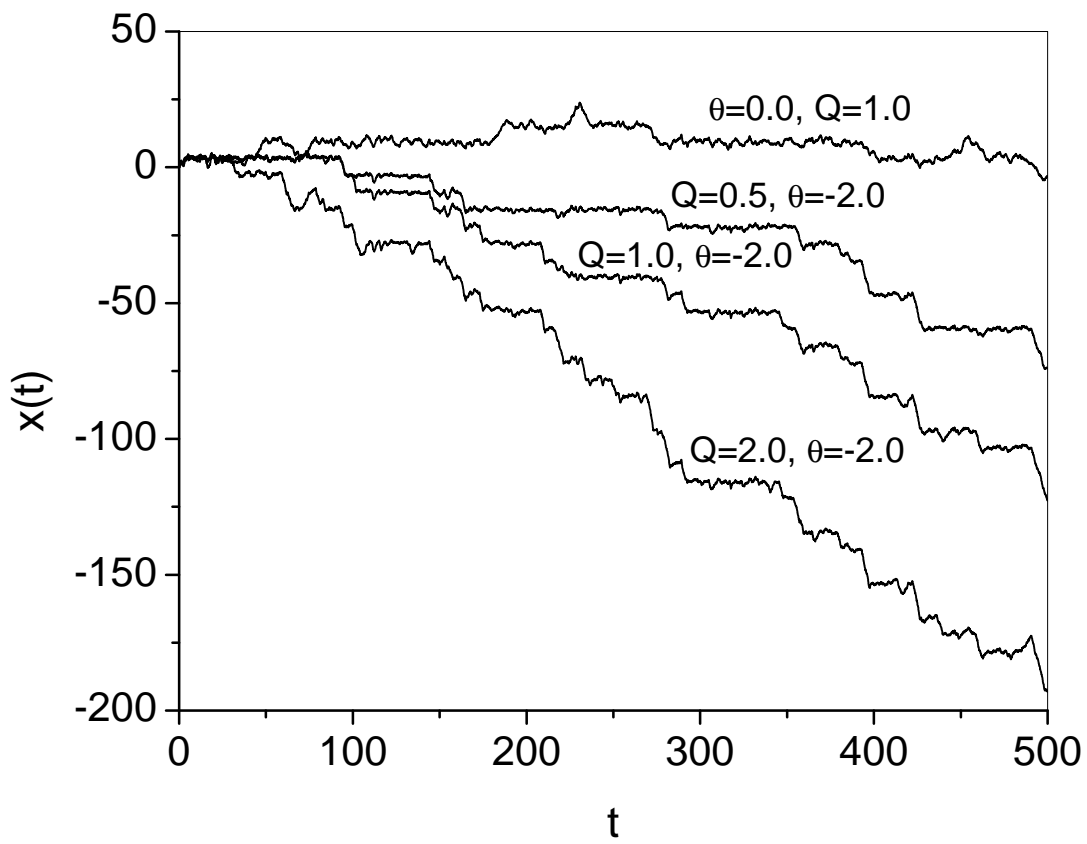


Fig.3

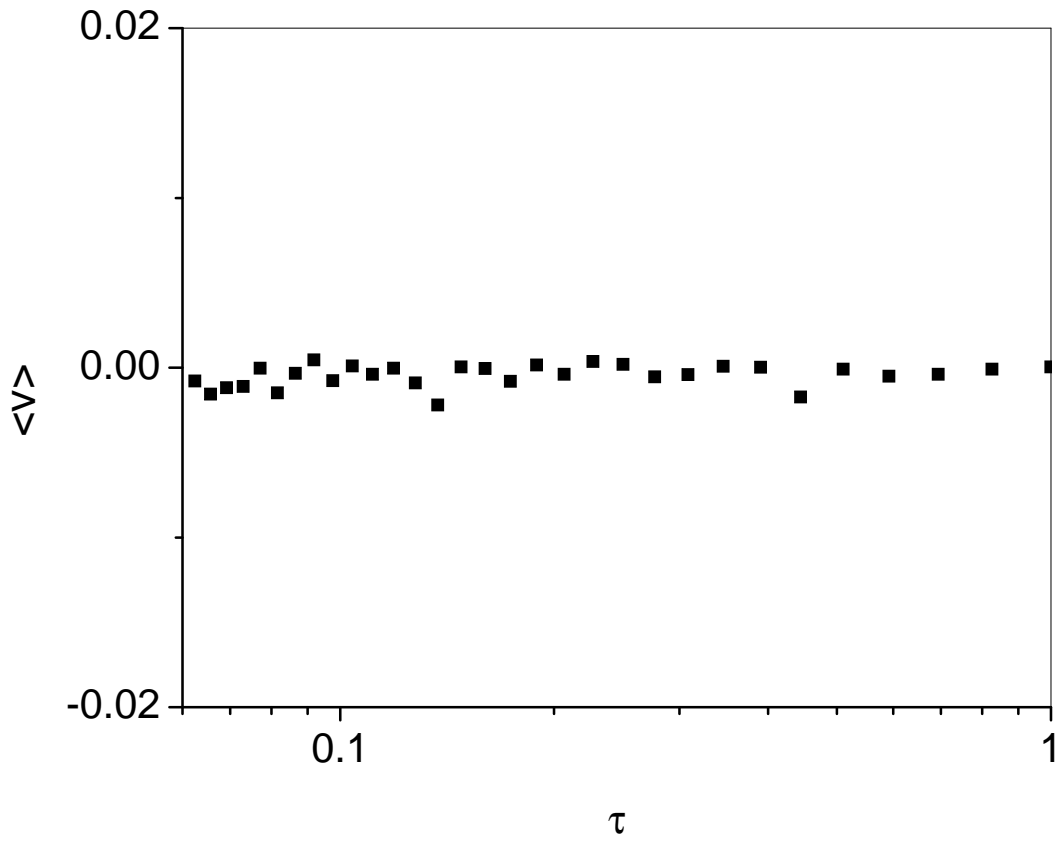


Fig.4

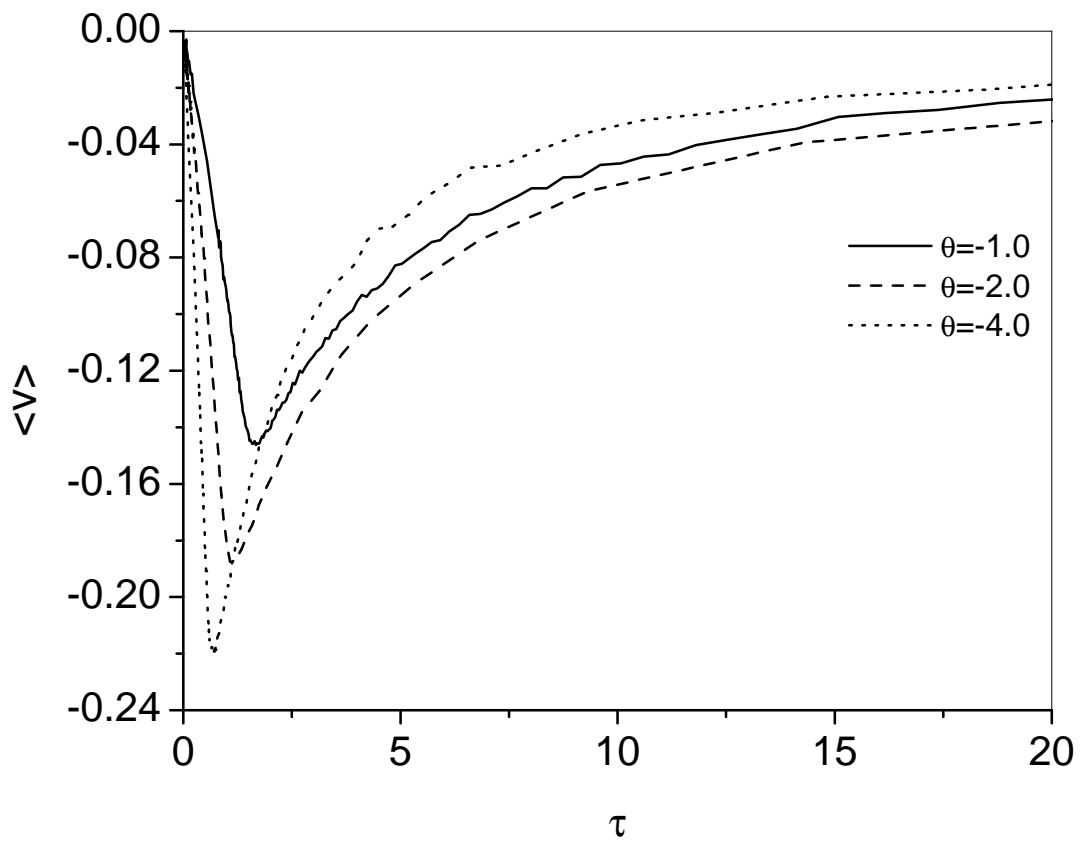


Fig.5

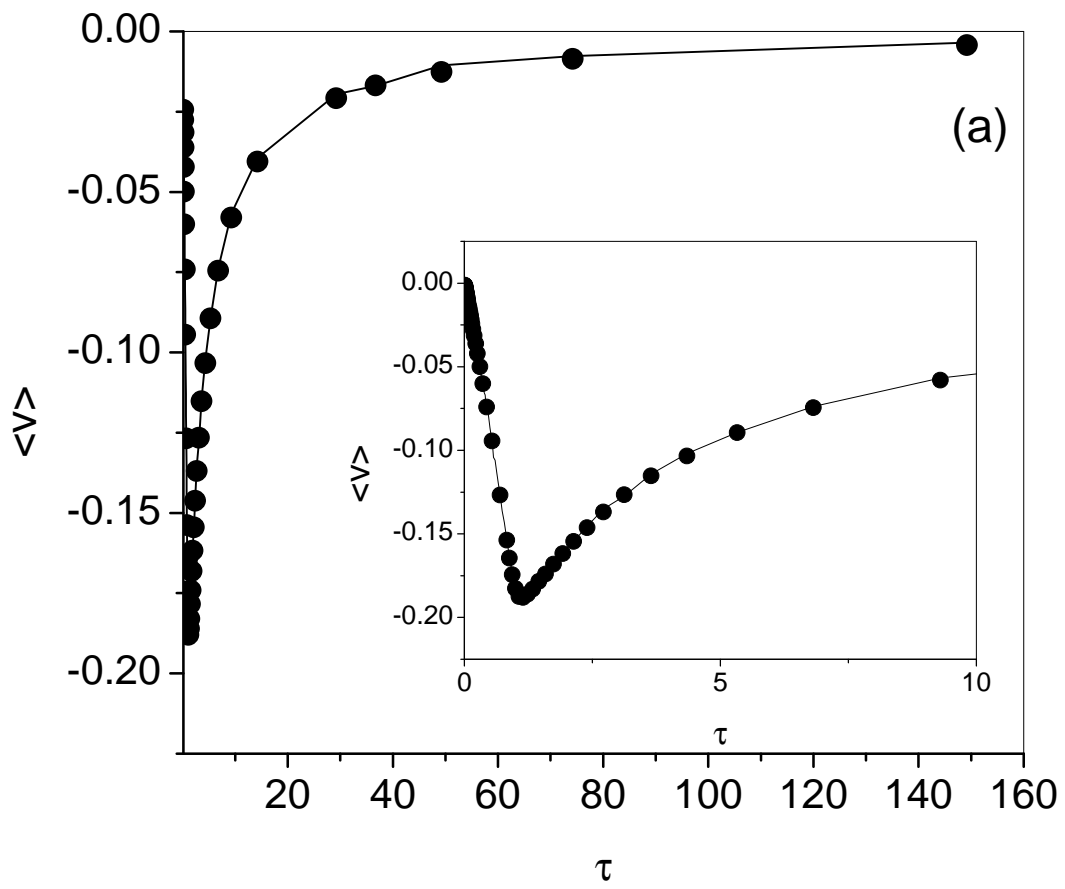


Fig.6

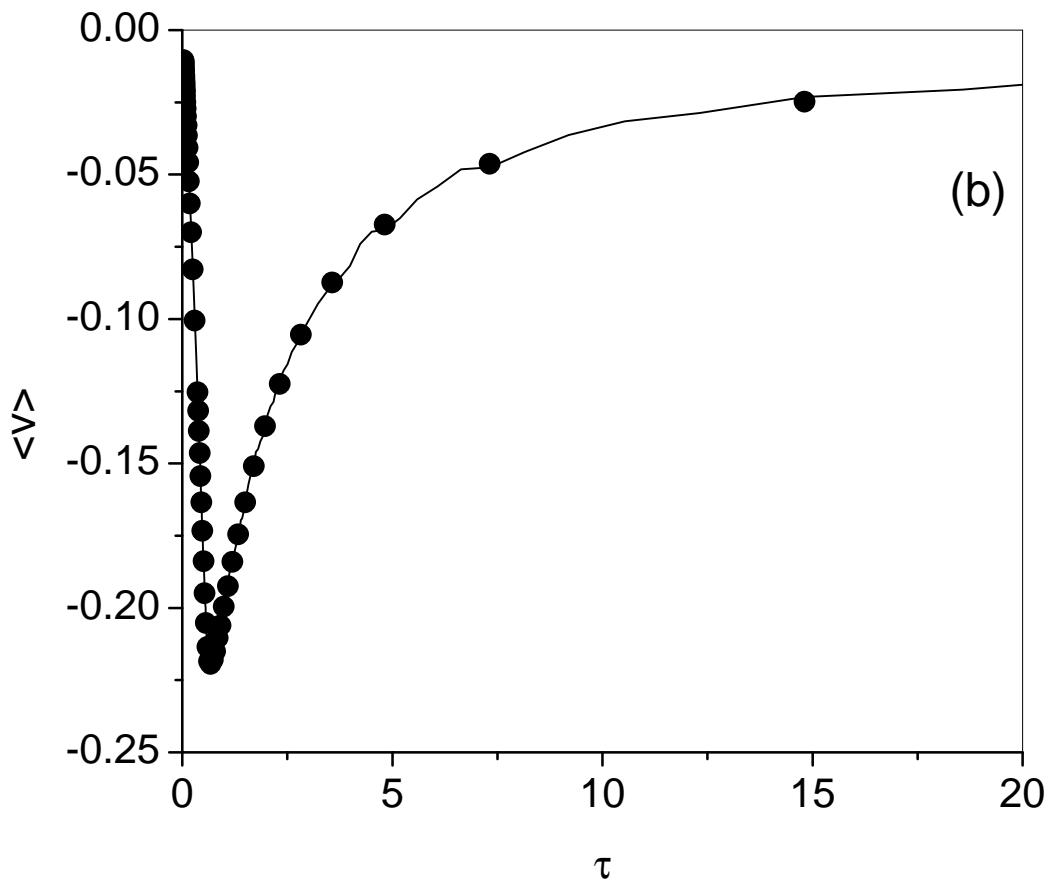


Fig.6

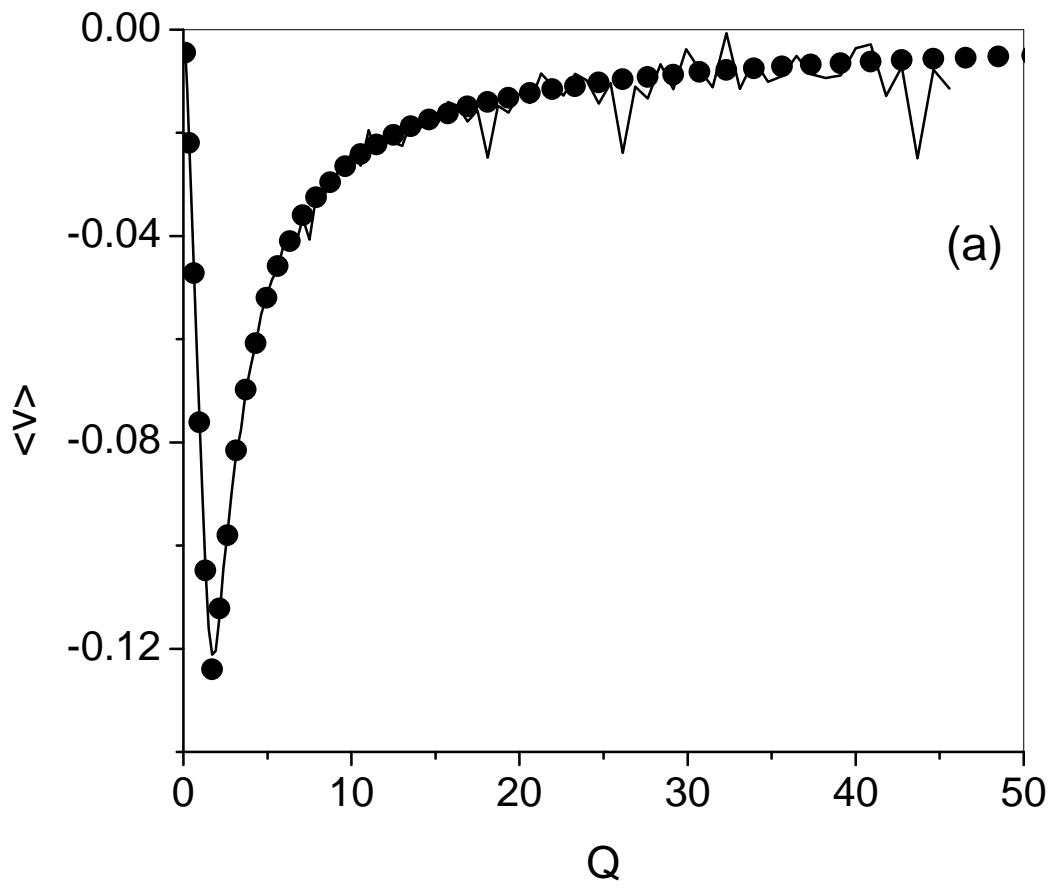


Fig.7

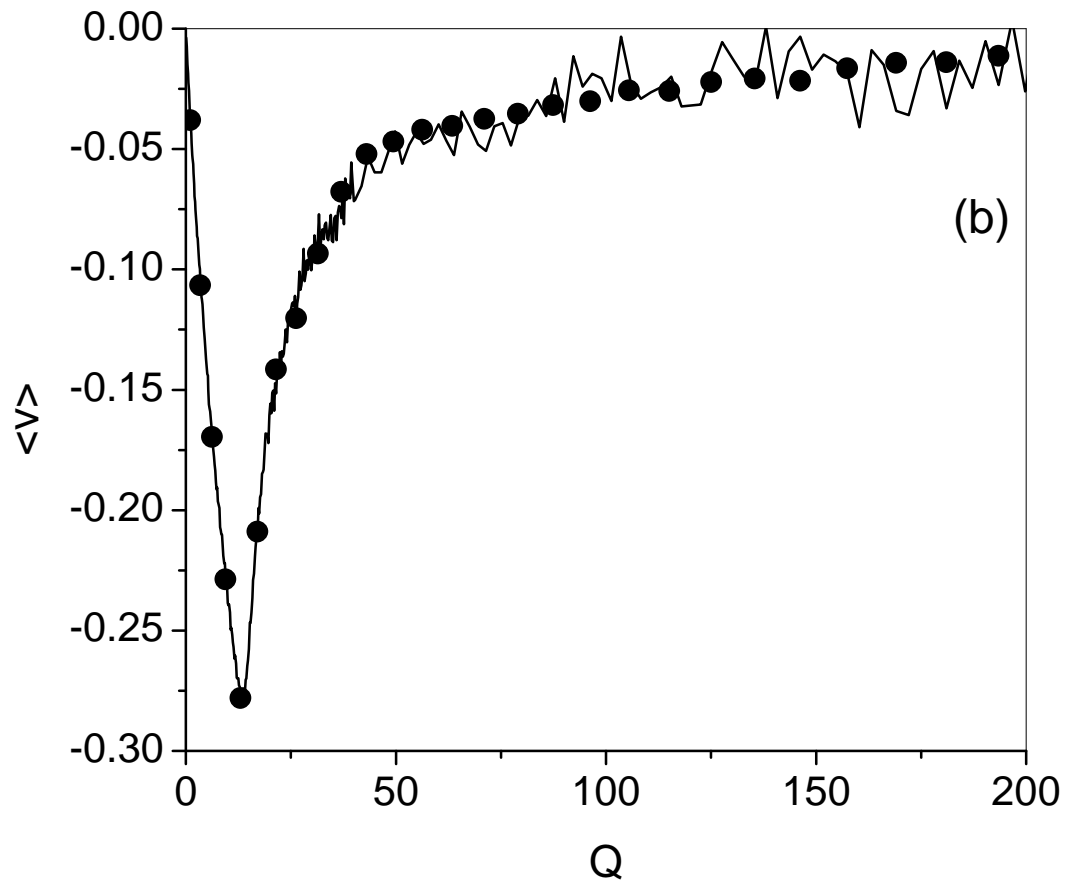


Fig.7

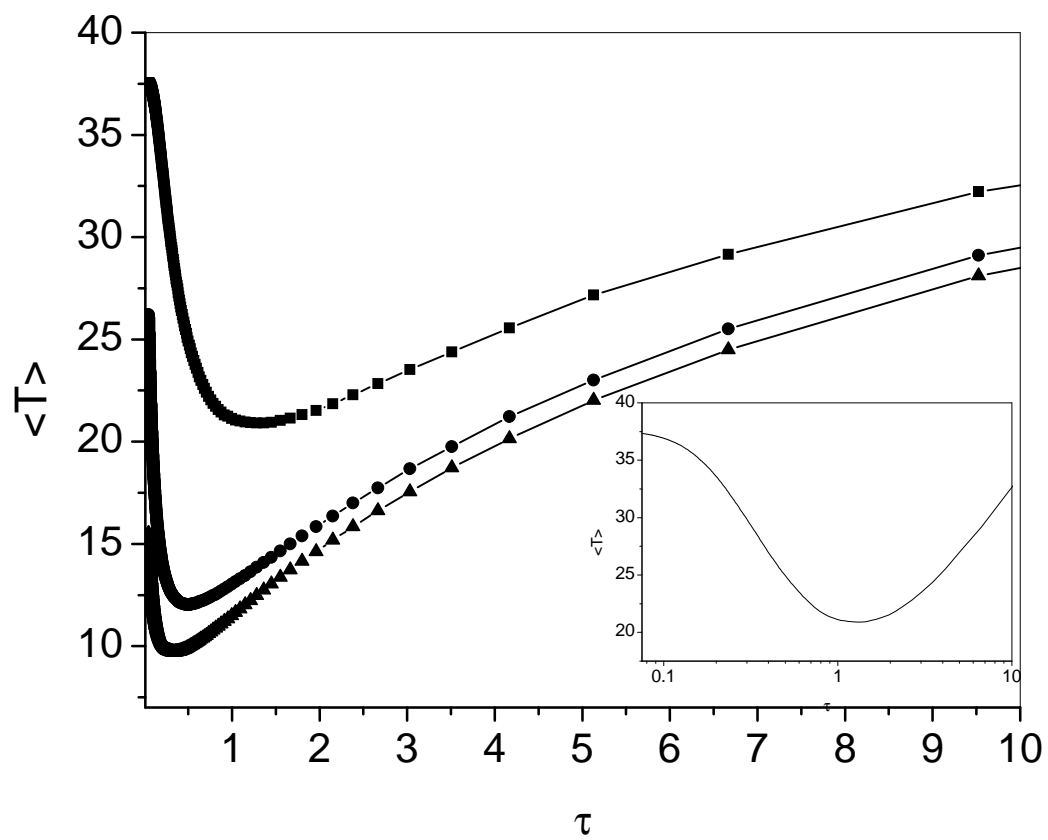


Fig.8

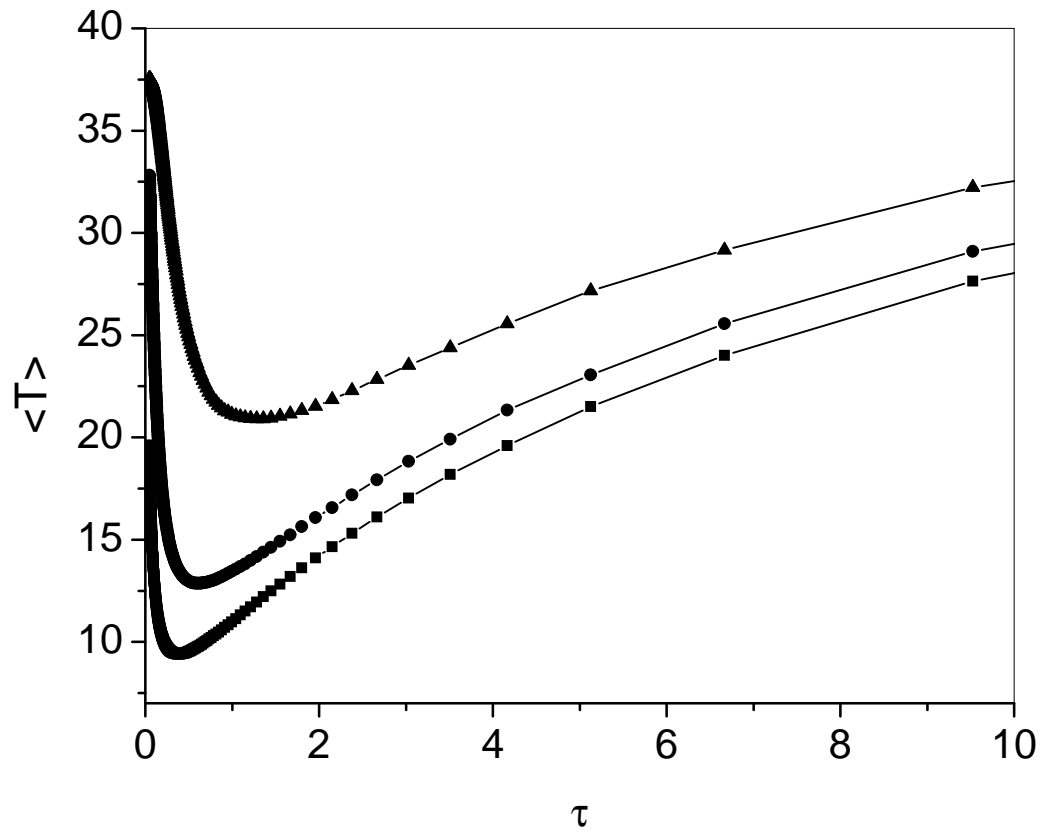


Fig.9