CHAPTER V

FORD-KAC-MAZUR MODEL

5.1 Introduction

In the previous sections we dealt with the analysis of average displacement and velocity for Brownian particle, which analysis satisfies mathematicians, but not physicists (9), that at present physicists try to derive the behavior of the particle from the law of dynamics only, and coupled harmonic oscillators is one of the models which are mathematically tractable and exhibit salient features.

In 1964, Ford, Kac, Mazur studied the motion of a particle of mass equal to the bath particle and found that the particle attains Brownian motion when the interaction is a very special long range type with a limiting frequency. To obtain the result they used a simple mechanical model, a chain of coupled harmonic oscillators. With this model they got a deeper understanding of some phenomena associated with Brownian motion. This model is later called " Ford-Kac-Mazur model(10)".

They used this model to carry through the program one would like to achieve with more realistic interactions. This program goes as follows.

(1) Solve the equations of motion of the system consisting of a Brownian particle coupled to heat bath. The solution consists of expressions for the coordinates and momenta at time t in terms of the initial coordinates and momenta.

(2) Assume the initial coordinates and momenta of the heat bath to be distributed as the canonical distribution.

(3) Show that the coordinate and momentum of the Brownian particle, as functions of time, will represent stochastic processes, whose statistically properties arise from the initial distribution of the heat bath. The processes are the kind from standard theories. This is an ambitious program, so it can be carried out only for the simplest models.

They know what the results of this program should be, since, Brownian motion is a throughly studied experimentally and theoretically. They expect to show the following results.

(1) The approach to equilibrium, that the momentum distribution of the Brownian particle should approach Maxwellian distribution (8,11).

(2) The description of this approach to equilibrium should be contracted, such that it should involve only a small number of the variables describing the system. The other way of saying is that there should be a reduced description of the stochastic process to be Markoff process.

We can be more explicit about what they mean by a contracted description of Brownian motion; they mean Langevin equation of motion.

For a Brownian particle of mass m acted upon by an external force F(x) this equation is

$$\dot{p} = - f p/m + E(t) + F(x) \tag{174}$$

where $p = m\dot{x}$ is the momentum of the particle, f the friction constant, and E(t) is the random force due to heat bath. This random force is a purely random gaussian process and has the properties (8)

$$\langle E(t)\, E(t+T) \rangle = 2 f k T \delta(t - t') \;;\; t' = t + T$$

where T is the temperature of the heat bath and k is Boltzmann's constant.

The Langevin equation is a contracted description in the sence that

(1) The heat bath is described by only two parameters, f and T

(2) Only the second derivative of the position x of the Brownian particle appears.

5.2 The model (10)

(I) Dynamics of a system of coupled oscillators (12)

Consider a system of (2N + 1) coupled oscillators; the Hamiltonian of the system is

$$H = \frac{1}{2}\sum_{j=-N}^{N} p_j^2 + \frac{1}{2}\sum_{j,k=-N}^{N} q_j A_{jk} q_k \tag{175}$$

where q_j and p_j ; are the canonical coordinate and momentum of the j-th oscillator.

The mass of each oscillator is equal to unity. The interactions of the oscillators are characterized by the (2N + 1) x (2N + 1) symmetric matrix $\bar{A}$, whose elements are A_{jk}. Assumed that this matrix $\bar{A}$ has no negative eigenvalues. The canonical equations of motion will be written in matrix notations as follows (12)

$$\dot{\bar{q}} = \bar{p} \,, \qquad \dot{\bar{p}} = -\bar{A}\bar{q} \tag{176}$$

where $\bar{p}$ and $\bar{q}$ are (2N + 1) rowed column matrices whose elements are p_j and q_j.

The formal solution of Eq.(176) is

$$\bar{q}(t) = \cos(\bar{A}^{1/2}t)\,\bar{q}(0) + \bar{A}^{-1/2}\sin(\bar{A}^{1/2}t)\,\bar{p}(0) \tag{177}$$

$$\bar{p}(t) = -\bar{A}^{1/2}\sin(\bar{A}^{1/2}t)\bar{q}(0) + \cos(\bar{A}^{1/2}t)\bar{p}(0) \tag{178}$$

We now assume that at t = o the system is in equilibrium at temperature T, therefore $q_j(0)$ and $p_j(0)$ are distributed according to the canonical distribution (8).

(6)

$$D(\bar{q}(0), \bar{p}(0)) = (2\pi/\beta)^{2N+1}(\det\bar{A})^{-1/2} e^{-\beta H(\bar{q}(0), \bar{p}(0))} \tag{179}$$

where $\beta = (kT)^{-1}$ and $\det\bar{A}$ is the determinant of $\bar{A}$. There is a difficulty in (179), since $\det\bar{A}=0$ if $\bar{A}$ has zero eigenvalues. We therefore assume that $\bar{A}$ has no zero eigenvalues. The expectation value of any function $F(\bar{q}(0), \bar{p}(0))$ is given by

$$\langle F\rangle = \int \cdots \int dq_{-N}(0) \cdots dq_{N}(0)\, dp_{-N}(0) \cdots dp_{N}(0) \times F(\bar{q}(0), \bar{p}(0))\, D(\bar{q}(0), \bar{p}(0)) \tag{180}$$

Now, what are the properties of the stochastic variables $q_j(t)$ and $p_j(t)$ from Eq. (177) under the canonical distribution.

First of all, it is clear that the process is gaussian (8), since the distribution (179) is gaussian. That the process is stationary, then it follows from the Liouville theorem of mechanics (12) that

$$D(\bar{q}(t), \bar{p}(t)) = D(\bar{q}(0), \bar{p}(0)) \tag{181}$$

That, the statistical properties of a stationary gaussian process are completely described by the pair correlation functions(8). From Appendix III, we obtain

$$\langle p_j(t)\, p_k(t+\tau)\rangle = kT\, \|\cos \bar{A}^{1/2}\tau\|_{jk} \tag{182.1}$$

$$\langle q_j(t)\, p_k(t+\tau)\rangle = -kT\, \|\bar{A}^{-1/2}\sin \bar{A}^{1/2}\tau\|_{jk} \tag{182.2}$$

$$\langle q_j(t)\, q_k(t+\tau)\rangle = kT\, \|\bar{A}^{-1}\cos \bar{A}^{1/2}\tau\|_{jk} \tag{182.3}$$

where $\bar{A}$ is the matrix A and $\|\bar{A}\|_{jk}$ is the j-th rowed and k-th columned element of the matrix A .

Note that the position correlation (182.3) involves the inverse of $\bar{A}$, which does not exist if $\bar{A}$ has zero eigenvalues

For a single oscillator, with index 0, the momentum autocorrelation (182.1) is

$$\langle p_0(t)\, p_0(t+\tau)\rangle = kT\, \|\cos \bar{A}^{1/2}\tau\|_{00} \tag{183}$$

This is the autocorrelation of a stationary gaussian process in one variable, and it is well known that such a process is Markoffian if and only if the autocorrelation (8) is an exponential, i.e,

$$\langle p_0(t)\, p_0(t+\tau)\rangle = kT\exp(-f|\tau|) \tag{184}$$

where f is a positive constant. The question we turn to next is that of finding an interaction matrix $\bar{A}$ for which Eq.(183) assumes the form Eq.(184)

(II) The interaction matrix (10)

In this model we assume the (2N + 1) oscillators are identical and arranged in a chain with cyclic boundary conditions. This means that the interaction matrix $\bar{A}$ is a symmetric cyclic matrix. The elements of such a matrix can be written in the form

$$A_{mn} = \frac{1}{2N+1}\sum_{k=-N}^{N} \omega_k^2 \exp\left\{ i\,\frac{2\pi}{2N+1}\,k(m-n)\right\} \tag{185}$$

With this formula we can readily demonstrate that $F(\bar{A})$ is a function of the matrix $\bar{A}$, then

$$\|F(\bar{A})\|_{mn} = \frac{1}{2N+1} \sum_{k=-N}^{N} F(\omega_k^2) \exp\left\{ i \frac{2\pi}{2N+1} k(m-n) \right\} \tag{186}$$

Consider next the limit $N \to \infty$, the infinite chain. If we assume that ω_s^2 is slowly varying function of s., then Eq.(185) becomes

$$A_{mn} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, f(\theta) \, e^{i(m-n)\theta}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, f(\theta) \cos(m-n)\theta \tag{187}$$

where

$$f(\theta) = \left\{ \omega_s^2 \right\}_{s=(2N+1)\theta/2\pi} \tag{188}$$

The relation (186) becomes in this limit ($N \to \infty$)

$$\|F(A)\|_{mn} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, F(f(\theta)) \cos(m-n)\theta \tag{189}$$

We now turn to the problem posed at the end of the last section; that of finding an interaction matrix $\bar{A}$ for which

$$\|\cos(\bar{A}^{1/2} t)\|_{00} = e^{-f|t|} \tag{190}$$

Using the result (186) we see that for a finite matrix

$$\|\cos \bar{A}^{1/2} t\|_{00} = \frac{1}{2N+1} \sum_{k=-N}^{N} \cos \omega_k t \tag{191}$$

For any choice of ω_k this is a quasiperiodic function and cannot be of the form Eq.(190). However, in the limit of large N, we can use Eq.(189)

which gives.

$$e^{-f|t|} = \|\cos A^{-1/2} t\|_{00} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \cos\left\{[f(\theta)]^{1/2} t\right\} \tag{192}$$

This becomes an integral equation for $f(\theta)$. The solution is

$$f(\theta) = f^2 \tan^2(\theta/2) \tag{193}$$

But, when Eq.(193) is inserted in equation (187) for the matrix element, the expression diverges. Therefore, we have to employ a second limiting process, defining

$$f_{\omega_L}(\theta) = \begin{cases} f^2 \tan^2 \theta/2, & |\theta| < \theta_L \\ 0, & \theta_L \leq |\theta| \leq \pi \end{cases} \tag{194}$$

where

$$\omega_L = f \tan \theta_L/2 \tag{195}$$

is a high-frequency cutoff in the spectrum of eigenfrequencies which ensures that the matrix element (187) are finite. This frequency cutoff corresponds to a "microscopic interaction time" ω_L^{-1} which is assumed to be very small compared to the "macroscopic relaxation time" f^{-1}. Therefore the result (190) holds only in the limit $\omega_L \to \infty$ or alternatively we can say that, for $\omega_L \gg f$ the result (190) holds for times long compared with ω_L^{-1}.

From Eq.(192), we make the change of veriable $\omega = f \tan\frac{\theta}{2}$, and use the result of the interaction matrix elements given in Eq.(187) with $f(\theta)$ given in Eq.(194) with $\omega_L \gg f$, we find

$$\|\cos A^{-1/2} t\|_{00} = \frac{1}{\pi}\int_{-\omega_L}^{\omega_L} d\omega \, \frac{f}{\omega^2 + f^2} \cos \omega t \tag{196}$$

For $\omega_L \to \infty$, the right-hand side of **Eq.**(196) (23) becomes $e^{-\gamma_0 |t|}$ and therefore, the gaussian process $\bar{p}_0(t)$ becomes also Markoffian.

III The Langevin equation (10)

We have shown in the preceding section that this model leads to a gaussian Markoffian stochastic process (6,8) for the collection of coupled oscillators, we are next investigate whether it leads to the Langevin equation for the motion of a single particle coupled to a heat bath consisting of such oscillators.

We indicate from the chain of (2N + 1) oscillators, the particle with index zero, to be the Brownian particle; and the remaining 2N oscillators represents the heat bath. The outside force acts on this particle is denoted by

$$F(t) = F(q_0(t)) \tag{197}$$

If we define $\bar{F}(t)$ to be a (2N + 1) - rowed column matrix whose elements are all zero except for the zero-th element which is $F(t)$, then the equation of motion for coupled "particle and heat bath" are

$$\dot{\bar{q}} = \bar{p} \; ; \quad \dot{\bar{p}} = -\bar{A}\bar{q} + \bar{F}(t) \tag{198}$$

of which the solutions are

$$\bar{q}(t) = \cos(\bar{A}^{1/2}t)\,\bar{q}(0) + \bar{A}^{-1/2}\sin(\bar{A}^{1/2}t)\,\bar{p}(0) + \int_0^t dt'\,\sin(\bar{A}^{1/2}(t-t'))\,\bar{F}(t')/\bar{A}^{1/2} \tag{199}$$

$$\bar{p}(t) = -\bar{A}^{1/2}\sin(\bar{A}^{1/2}t)\,\bar{q}(0) + \cos(\bar{A}^{1/2}t)\,\bar{p}(0) + \int_0^t dt'\,\cos(\bar{A}^{1/2}(t-t'))\,\bar{F}(t') \tag{200}$$

If we take the zeroth element of Eq.(198) for $\dot{\bar{p}}$, and use $\bar{q}(t)$ in Eq.(199) we get

$$\dot{p}_0 = -\sum_j \|\bar{A}\cos\bar{A}^{1/2}t\|_{0j}\, q_j(0) - \sum_j \|\bar{A}^{1/2}\sin\bar{A}^{1/2}t\|_{0j}\, p_j(0) - \int_0^t dt'\, \|\bar{A}^{1/2}\sin\bar{A}^{1/2}(t-t')\|_{00}\, F(t') + F(t) \quad (201)$$

The result (201) can be written in the form

$$\dot{p}_0 - F(t) = -\gamma(t)\, p_0 + E(t) + \int_0^t dt'\{\gamma(t) - \gamma(t-t')\} \times \|\cos\bar{A}^{1/2}(t-t')\|_{00}\, F(t') \quad (202)$$

where

$$\gamma(t) = \frac{\|\bar{A}^{1/2}\sin\bar{A}^{1/2}t\|_{00}}{\|\cos\bar{A}^{1/2}t\|_{00}} = -\frac{d}{dt}\ln\|\cos\bar{A}^{1/2}t\|_{00} \quad (203)$$

and

$$E(t) = -\sum_j\left\{\gamma(t)\, \|\bar{A}^{1/2}\sin\bar{A}^{1/2}t\|_{0j} + \|\bar{A}\cos\bar{A}^{1/2}t\|_{0j}\right\} q_j(0) + \sum_j\left\{\gamma(t)\, \|\cos\bar{A}^{1/2}t\|_{0j} - \|\bar{A}^{1/2}\sin\bar{A}^{1/2}t\|_{0j}\right\} p_j(0) \quad (204)$$

Eq.(202) is the equation of motion for the Brownian particle. The right-hand side is the net force exerted on the Brownian particle by the heat bath. The first term represents a frictional force with time dependent "friction coefficient" $\gamma(t)$, the second term represents a fluctuating force $E(t)$ depending on the initial state of the heat bath $(q_j(0),\ p_j(0))$, and the third term represents a memory effect depending on the past history of the motion of the Brownian particle.

From Eqs (196) and (203) we find that

$$\lim \gamma(t) = f \tag{205}$$

which is a constant

This implies that the last term on the right hand side of Eq.(202) which is the memory-effect term becomes, in the limit, equals to zero (because $\gamma(t) = \gamma(t - t') = f$)

With this results, Eq.(202) takes the form

$$\dot{p}_0 - F(t) = -f p_0 + E(t) \tag{206}$$

with

$$\begin{aligned} E(t) = & -\sum_j \| f \bar{A}^{-1/2} \sin \bar{A}^{-1/2} t + \bar{A} \cos \bar{A}^{-1/2} t \|_{0j}\, q_j(0) \\ & + \sum_j \| f \cos \bar{A}^{-1/2} t - \bar{A}^{-1/2} \sin \bar{A}^{-1/2} t \|_{0j}\, p_j(0) \end{aligned} \tag{207}$$

Equation (206) is the Langevin equation. Then, this model leads to Langevin equation as expected.

IV The statistical distribution of E(t)(10)

It remains to prove that the statistical properties of E(t)(8) becomes a purely random gaussian process in the limit $N \to \infty, \omega_L \gg f$.
Let at t = o, the heat bath is in equilibrium at temperature T and assume that the initial distribution is the canonical distribution and assume that the interaction between the Brownian particle and the heat bath is invariant under translations, that $\sum_j A_{ij} = 0$.
The latter assumption implies that $\omega_0 = 0$ so that $\det \bar{A} = 0$ and canonical distribution assumed becomes improper. This difficulty can be remedied by slightly modifying the matrix $\bar{A}$ by

$$\bar{A} + \varepsilon_N \bar{I} \tag{208}$$

where ε_N is positive for every finite N and approaches zero as $N \to \infty$ as fast as one pleases.

Therefore, $\sum_j A_{ij} = o$, is only approximately true and the canonical distribution is proper.

Since the distribution of $q_j(o)$, and $p_j(o)$ is gaussian, $E(t)$ is a gaussian process. With the help of the results in Appendix III , we find that

$$\langle E(t)E(t')\rangle = kT \,\|(f^2+\bar{A}) \cos \bar{A}^{1/2}(t-t')\|_{00} \tag{209}$$

From Eq.(209), using Eq.(189), we find

$$\begin{aligned}\langle E(t)E(t')\rangle &= \frac{kT}{2\pi}\int_{-\pi}^{\pi} d\theta \left(f^2 + f^2\tan^2\frac{\theta}{2}\right) \cos f \tan\frac{\theta}{2}(t-t') \\ &= \frac{kTf}{\pi}\int_{-\infty}^{\infty} d\omega \cos\omega(t-t')\end{aligned} \tag{210}$$

The integral in Eq.(210) is the well-known expression of Dirac delta function, so we have as expected

$$\langle E(t)E(t')\rangle = 2fkT\,\delta(t-t') \tag{211}$$

Thus $E(t)$ is a purely random, gaussian, stochastic process (8).

It is striking that the equation of motion (202) becomes Langevin equation when

(i) the friction constant $\gamma(t)$ be independent of time

(ii) $E(t)$ is a purely random gaussian stochastic process.

(iii) the memory effects disappear

We can see that these three properties are the intimate relation. This model is, therefore, proved to be satisfactory dynamical model representing Brownian motion of a particle.