DYNAMICAL THEORIES OF BROWNIAN MOTION

J. T. Lewis*
DIAS, Dublin 4, Republic of Ireland
and
J. V. Pulè
Royal University, Malta.

1. Introduction

Nelson (1) has shown how to derive the Einstein-Smolucnowski theory of Brownian motion from the Ornstein-Uhlenbeck theory which starts from the Langevin equations on phase space. We aim to derive the Ornstein-Uhlenbeck theory from the Maxwell-Boltzmann theory by making a mechanical model of the stationary Ornstein-Uhlenbeck process. The essential ideas of this treatment are contained in the paper of Ford, Kac and Mazur (2), but our treatment lays emphasis on the underlying mathematical structure. The case in which the restoring force is linear in the displacement has been considered in (3) where the connection with (2) is spelt out.

2. Dynamics of a Conservative Linear System (4)

We take the phase space of the system to be a real vector space Γ_1 and suppose that the total energy $E(\gamma)$ of the system corresponding to the state $\gamma \in \Gamma_1$ is given by $E(\gamma) = mc^2 H(\gamma)$ where $\gamma \to H(\gamma)$ is a strictly positive quadratic form on Γ_1, and mc^2 has the dimensions of energy. Choose a norm $|\cdot|$ on Γ_1 by putting $|\gamma|^2 = 2H(\gamma)$. Let Γ be the completion of Γ_1 with respect to the metric got from $|\cdot|$, so that Γ is a Hilbert space with inner product $<\cdot, \cdot>$ given by $2<\gamma_1, \gamma_2> = |\gamma_1 + \gamma_2|^2 - |\gamma_1|^2 - |\gamma_2|^2$. Let $t \to \gamma_t = T_t\gamma$ be a flow on Γ leaving H invariant. Then there is a linear operator D on a dense domain in which is skew-symmetric with respect to the inner product and is such that $T_t = \exp(tD)$. Assume that $-D^2$ is strictly positive (it is certainly non-negative since $-D^2 = D^*D$). Then D can be written uniquely as JA where J is a complex structure and A is strictly positive. Then for γ in the domain of D we have

$$\frac{d}{dt}\gamma_t = JA\gamma_t \quad . \tag{2.1}$$

There is a pair E, F of closed subspaces of Γ invariant under exp(-tA)

*Speaker

($t > 0$) such that $F = JE$ and $\Gamma = E + F$. When $\dim \Gamma = 2n < \infty$ there is an orthonormal basis $\{e_i: i = 1, .., n\}$ for E such that $Ae_i = \alpha_i e_i$; then $\{f_i = Je_i: i = 1, .., n\}$ is an orthonormal basis for F and $Af_i = \alpha_i f_i$. Putting $Q^i_t(\gamma) = \langle e_i, T^*_t\gamma\rangle$ and $P^i_t(\gamma) = \langle f_i, T^*_t\gamma\rangle$ we find that (2.1) yields

$$\frac{d}{dt} Q^i_t(\gamma) = \alpha_i P^i_t(\gamma) \quad \frac{d}{dt} P^i_t(\gamma) = -\alpha_i Q^i_t(\gamma) , \tag{2.2}$$

3. Dynamics of Dissipative Linear Systems

The dissipative linear systems we consider are got from conservative linear systems by adding a damping term to the generator: let Γ, H, T_t be as in 2, let B be an operator commuting with J such that B is zero on E and strictly positive on F, put $G = JA - B$ and $S_t = \exp(tG)$, $t \geqslant 0$.

LEMMA. $\{S_t: t > 0\}$ *is a strongly continuous semi-group of contractions on* Γ *such that* $S_t x \to 0$ *as* $t \to \infty$ *for each* x *in* Γ .

Suppose that $\dim \Gamma = 2n < \infty$ and, with the notation of 2, put $\beta_{ij} = \langle f_i, Bf_j\rangle$ and $Q^i_t(\gamma) = \langle S_t e_i, \gamma\rangle$, $P^i_t(\gamma) = \langle S_t f_i, \gamma\rangle$; then

$$\frac{d}{dt} Q^i_t = \alpha_i P^i_t , \quad \frac{d}{dt} P^i_t = -\alpha_i Q^i_t - \sum_j \beta_{ij} P^i_t , \quad t > 0 . \tag{3.1}$$

We see that our assumptions about S_t amount to the inclusion in the equations of motion of phenomenological damping terms linear in the velocities. Such terms arise in Stoke's theory of viscous damping and in Rayleigh's theory of Doppler drag.

4. Embedding Dissipative Linear Systems

Can a dissipative linear system Γ^0, H^0, $S_t = \exp(tG)$ be embedded isometrically in a conservative linear system Γ, H, T_t in such a way that the flow S_t is the restriction of the flow T_t to Γ^0 ? This is answered in the affirmative by the following version of the Sz.-Nagy Dilation Theorem:

THEOREM 1 (see (4), (5) and (6)) *Let* $\Gamma^0 = E^0 + F^0$ *be a phase space with dissipative flow* $S_t = \exp(tG)$, $G = J^0A^0 - B$. *Then there exists an isometric embedding* $j: \Gamma^0 \to \Gamma\ L^2(R; F^0)$, *a conservative flow* $T_t = \exp(tJA)$ *on* Γ *and a projection* P *on* Γ *such that* $j \circ S_t = PT_t \circ j$.

Sketch of proof: let $(T_t f)(s) = f(s - t)$,

$$(Pf)(s) = \begin{cases} f(s) & , s < 0, \\ 0 & , s > 0, \end{cases} \quad \text{and} \quad (jx)(s) = \begin{cases} (2B)^{\frac{1}{2}} S_{-s} x & , s < 0, \\ 0 & s > 0. \end{cases}$$

Warning: $j\,\Gamma^0$ is not contained in D(JA) and subsequent computations depend crucially on the following theorem:

THEOREM 2 (see (6)) *For every* x *in* $D(G) \subset \Gamma^0$ *we have*

$$(T_t \circ jx)(\cdot) = (jx)(\cdot) + \int_0^t (T_s \circ jGx)(\cdot)ds + \chi_{(o,t)}(\cdot)\,(2B)^{\frac{1}{2}}\,x.$$

Using the notation of 3 in the case where $\dim \Gamma^0 = 2$ but this time putting $Q_t(\gamma) = \langle je, T_t^* \gamma\rangle$, $P_t(\gamma) = \langle jf, T_t^* \gamma\rangle$ we have

$$\frac{dQ}{dt} = \alpha P_t \ , \ \frac{dP}{dt}t = -\alpha Q_t - \beta P_t + (2\beta)^{\frac{1}{2}}\,\gamma(t)$$

Here the damping term arises from the flow of energy into the reservoir whose phase space is $(j\Gamma^0)^{\perp}$. In addition there is a driving term which leads us to identify the function $t \to \gamma(t)$, $t > 0$, with the future history of the driving of the system by the reservoir.

5. Embedding a Dissipative Non-Linear System

Consider a non-linear system with equations of motion

$$\frac{d}{dt}\overline{Q}_t = \alpha\overline{P}_t, \quad \frac{d\overline{P}}{dt}t = -\alpha\overline{Q}_t - \beta\,\overline{P}_t - \alpha\,V'(\overline{Q}_t). \tag{5.1}$$

We embed it in a conservative system by perturbing the linear system used in 4. Put $\overline{Q}_t(\gamma) = \langle je, \overline{T}_t\gamma\rangle$, $\overline{P}_t(\gamma) = \langle f, \overline{T}_t\gamma\rangle$ where $t \to \overline{T}_t\gamma$ is the non-linear flow on Γ given by

$$\overline{T}_t\,\gamma = T_t^*\,\gamma - \int_0^t T_{t-s}^* \circ jGe\,V'(\langle je, \overline{T}_s\gamma\rangle)\,ds \quad . \tag{5.2}$$

(Standard methods give the existence and uniqueness of this flow under appropriate conditions on V'.) Then we have

$$\frac{d\overline{Q}}{dt}t = \alpha\overline{P}_t \ , \ \frac{d\overline{P}}{dt}t = -\alpha\overline{Q}_t - \beta\overline{P}_t - \alpha V'(\overline{Q}_t) + (2\beta)^{\frac{1}{2}}\,\gamma(t) \tag{5.3}$$

and the flow $t \to \overline{T}_t$ preserves the total energy which is now given by

$$mc^2\,\{\tfrac{1}{2}\,|\gamma|^2 + V(\langle je,\gamma\rangle)\}.$$

6. *Statistical Mechanics of Linear Systems*

We return to the conservative systems considered in 2. When $\dim \Gamma = 2n < \infty$ the Maxwell-Boltzmann prescription puts a measure μ_T on Γ having density $(2\pi\ kT/mc^2)^{-n} \exp(-\ mc^2 H(\gamma)/kT)$ with respect to Lebesque measure. Then for each ξ in Γ we have $E \exp(i<\cdot,\xi>) = \int_\Gamma \exp(i<\gamma,\xi>) d\mu(\gamma) = \exp(-\frac{1}{2}\sigma^2 |\xi|^2)$ where $\sigma^2 = kT/mc^2$, so that $<\cdot,\xi>$ is a Gaussian random variable with $E<\cdot\ \xi> = 0$, $E <\cdot,\xi>^2 = \sigma^2|\xi|^2$. Thus for linear systems the Maxwell-Boltzmann prescription is entirely equivalent to the following: let Ω, P be a probability space and let $\phi : \Gamma \to L^2(\Omega, P)$ be a linear mapping such that for each ξ in Γ the random variable $\phi(\xi)$ is Gaussian with $E\ \phi(\xi) = 0$, $E\phi\ (\xi)^2 = \sigma^2\ |\xi|^2$. In this case, of course, we may take $\Omega = \Gamma$ and $P = \mu_T$. This prescription makes sense even when $\dim\Gamma = \infty$ and in this case we adopt it as the Maxwell-Boltzmann prescription, even though it is no longer possible to take $\Omega = \Gamma$. However in the situation described in 4 we have $\Gamma = L^2(R;\ F^0)$ and there is a unique probability measure μ_T on $\Gamma^* = \mathcal{S}'(R;F^0)$ such that, for each ξ in ${}_*\Gamma = \mathcal{S}(R;\ F^0)$, $E \exp(i<\cdot,\ \xi>) = \exp(-\ \frac{1}{2}\sigma^2|\xi|^2)$ where now $<x,\xi>$ is the pairing between Γ^* and ${}_*\Gamma$. We can take ϕ to be the unique continuous extension of the map $\xi \to <\cdot\ \xi>$ to a map from Γ to $L^2(\Gamma^*,\mu_T)$. T_t leaves ${}_*\Gamma$ invariant so its restriction ${}_*T_t$ is well-defined and induces an adjoint action T_t^* on Γ^*. Note that now $\phi(\cdot) = \sigma\ W(\cdot)$ where $W(\cdot)$ is the Wiener Stochastic Integral. (For a fuller account of all this see Hida (7).)

7. The Ornstein-Uhlenbeck Process

Returning to 4 we put $Q^t(x) = < T_t^* x, je>$, $P_t(x) = < T_t^* x, jf>$ and then we have

THEOREM 3 $Q_t(\cdot)$, $P_t(\cdot)$ *is a Gaussian stochastic process satisfying the Langevin equation*

$$dQ_t(\cdot) = \alpha P_t(\cdot),\quad dP_t(\cdot) = -\ \alpha Q_t(\cdot) - \beta P_t(\cdot) + (2\beta kT/mc^2)^{\frac{1}{2}}\ W_t(\cdot)$$

where $W_t(\cdot)$ *is a Wiener process such that* $EW_t = 0$, $EW_s W_t = \min(s,\ t)$.

References

(1) Nelson, E., Dynamical Theories of Brownian Motion, Princeton (1967)
(2) Ford, G. W., M. Kac and P. Mazur, J. M.P. 6,505-515 (1965)
(3) Lewis, J. T. and L. C. Thomas, Functional Integration, Oxford (1975)
(4) Lax, P. D. and R. S. Phillips, Scattering Theory, New York (1967)
(5) Sz.-Nagy, B. and C. Foias, Harmonic Analysis..., Amsterdam (1970)
(6) Lewis, J. T. and L.C. Thomas, Z. Wahrschein. 30, 45-55 (1974)
(7) Hida, T., Stationary Stochastic Processes, Princeton (1970)