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APPENDIX I

THE GENERAL PROBLEM OF RANDOM FLIGHTS; MARKOFF'S METHOD (6)

In the general problem of random flights, the position $\vec{R}$ of the particle after N displacements is given by

$$\vec{R} = \sum_{i=1}^{N} \vec{r}_i \tag{A-1}$$

where the $\vec{r}_i$'s $(i=1,\ldots,N)$ denote the different displacements. Further, the probability that the i displacement lies between $\vec{r}_i$ and $\vec{r}_i + d\vec{r}_i$ is given by

$$\tau_i(x_i, y_i, z_i)\, dx_i dy_i dz_i = \tau_i\, dr_i \;; (i=1,\ldots,N) \tag{A-2}$$

We require the probability $W_N(\vec{R})d\vec{R}$ that the position of the particle after N displacements lies in the interval $\vec{R}$, $\vec{R}+d\vec{R}$

Let

$$\vec{\phi}_j = (\phi_j^1, \phi_j^2, \ldots\ldots, \phi_j^n) \quad (j=1,\ldots,N) \tag{A-3}$$

be N, n-dimensional vectors, the components of each of these vectors being functions of s coordinates:

$$\phi_j^k = \phi_j^k(q_{j}^1, \ldots\ldots, q_{j}^s) \quad (k=1,\ldots,n\,; j=1,\ldots,N) \tag{A-4}$$

The probability that the q_j^i's occur in the range

$$q_j^1, q_j^1 + dq_j^1; q_j^2, q_j^2 + dq_j^2; \ldots\ldots; q_j^s, q_j^s + dq_j^s \tag{A-5}$$

is given by

$$\tau_j(q_j^1, \ldots\ldots, q_j^s)\, dq_j^1 \ldots dq_j^s = \tau_j(\vec{q}_j)\, d\vec{q}_j \tag{A-6}$$

Further, let

$$(\Phi^1, \Phi^2, \ldots\ldots, \Phi^n) = \vec{\Phi} = \sum_{j=1}^{N} \vec{\phi}_j \tag{A-7}$$

The problem is: What is the probability that

$$\vec{\Phi}_0 - \tfrac{1}{2} d\vec{\Phi}_0 \le \vec{\Phi} \le \vec{\Phi}_0 + \tfrac{1}{2} d\vec{\Phi}_0 \tag{A-8}$$

where $\vec{\Phi}_0$ is some preassigned value for $\vec{\Phi}$

If we denote the required probability by

$$W_N(\vec{\Phi}_0)d\Phi_0^1 \cdots d\Phi_0^n = W(\vec{\Phi}_0)d\vec{\Phi}_0 \tag{A-9}$$

we have

$$W_N(\vec{\Phi}_0)\,d\vec{\Phi}_0 = \int\cdots\int \prod_{j=1}^{N}\left\{\tau_j(\vec{q}_{\gamma j})\,d\vec{q}_{\gamma j}\right\} \tag{A-10}$$

where the integration is effected over only those parts of the N,s-dimensional configuration space $(q_{\gamma 1}^1, \ldots\ldots, q_{\gamma N}^s)$ in which the inequalities (A-8) are satisfied.

Introduce a factor $\Delta(\vec{q}_{\gamma 1}, \ldots, \vec{q}_{\gamma N})$ having the following properties:

$$\Delta(\vec{q}_{\gamma 1}, \ldots, \vec{q}_{\gamma N}) = 1 \quad \text{whenver} \quad \Phi_0 - \tfrac{1}{2}d\Phi_0 \leq \Phi \leq \Phi_0 + \tfrac{1}{2}d\Phi_0 \tag{A-11}$$

$$= 0 \quad \text{otherwise}$$

Then,

$$W_N(\vec{\Phi}_0)\,d\vec{\Phi}_0 = \int\cdots\int \Delta(\vec{q}_{\gamma 1}, \ldots, \vec{q}_{\gamma N})\prod_{j=1}^{N}\left\{\tau_j(\vec{q}_{\gamma j})\,d\vec{q}_{\gamma j}\right\} \tag{A-12}$$

Consider the integrals

$$\delta_k = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\sin \alpha_k \rho_k}{\rho_k}\, exp(i\,\rho_k \gamma_k)\, d\rho_k \quad (k=1,\ldots,n) \tag{A-13}$$

δ_k is the discontinuous integral of Dirichlet and has the property

$$\delta_k = 1 \quad \text{whenever} \quad -\alpha_k < \gamma_k < \alpha_k$$

$$= 0 \quad \text{otherwise} \tag{A-14}$$

Now, let

$$\alpha_k = \tfrac{1}{2}d\Phi_0^k, \quad \gamma_k = \sum_{j=1}^{N}\phi_j^k - \Phi_0^k \quad (k=1,\ldots,n) \tag{A-15}$$

According to Eq. (A-14)

$$\delta_k = 1 \quad \text{whenever} \quad \Phi_0^k - \tfrac{1}{2}d\Phi_0^k < \sum_{j=1}^{N}\phi_j^k < \Phi_0^k + \tfrac{1}{2}d\Phi_0^k \tag{A-16}$$

$$= 0 \quad \text{otherwise}$$

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Consequently

$$\Delta = \prod_{k=1}^{n} \delta_k \tag{A-17}$$

has the required properties (A-11)

Substituting for Δ from Eqs.(A-13) and (A-17) in Eq.(A-12) we obtain

$$W_N(\vec{\Phi}_0)\,d\vec{\Phi}_0 = \frac{1}{\pi^n}\int_{(\vec{\rho})}\cdots\int\int_{(\vec{q})}\cdots\int\left\{\prod_{j=1}^{N}\tau_j(\vec{q}_j)\,d\vec{q}_{bj}\right\}\left\{\prod_{k=1}^{n}\frac{\sin\left(\frac{1}{2}d\Phi_0^k\,\rho_k\right)}{\rho_k}\right\}$$
$$\times\exp\left\{i\left[\sum_{k=1}^{n}\sum_{j=1}^{N}\phi_j^k\,\rho_k - \sum_{k=1}^{n}\Phi_0^k\,\rho_k\right]\right\}d\rho_1\cdots d\rho_n \tag{A-18}$$
$$= \frac{d\vec{\Phi}_0}{2^n\pi^n}\int\cdots\int\exp(-i\vec{\rho}\cdot\vec{\Phi}_0)\,A_N(\vec{\rho})\,d\vec{\rho}$$

where

$$A_N(\vec{\rho}) = \prod_{j=1}^{N}\int\cdots\int dq_{bj}^1\cdots dq_{bj}^s\,\exp(i\vec{\rho}\cdot\vec{\phi}_j)\,\tau_j(q_{bj}^1,\ldots,q_{bj}^s) \tag{A-19}$$

The case of greatest interest is when all the functions τ_j are identical. Equation.(A-19) then becomes

$$A_N(\vec{\rho}) = \left[\int\exp(i\vec{\rho}\cdot\vec{\phi})\,\tau(\vec{q}_b)\,d\vec{q}_b\right]^N \tag{A-20}$$

According to Eq.(A-18) $A_N(\vec{\rho})$ is the n-dimensional Fourier-transform of the probability function $W(\vec{\Phi}_0)$

According to Eqs.(A-1), (A-18) and(A-19), the probability $W_N(\vec{R})\,d\vec{R}$

that the position $\vec{R}$ of the particle will be found in the interval $(\vec{R},\vec{R}+d\vec{R})$ after N displacements is given by

$$W_N(\vec{R}) = \frac{1}{8\pi^3}\int_{-\infty}^{\infty}\exp(-i\vec{\rho}\cdot\vec{R})\,A_N(\vec{\rho})\,d\vec{\rho} \tag{A-21}$$

where

$$A_N(\vec{\rho}) = \prod_{j=1}^{N}\int_{-\infty}^{\infty}\tau_j(\vec{r}_j)\,\exp(i\vec{\rho}\cdot\vec{r}_j)\,d\vec{r}_j \tag{A-22}$$

In Eq.(A-22) $\tau_j(\vec{r}_j)$ governs the probability of occurrence of a displacement $\vec{r}_j$ on the j-th occasion. The explicit form which W_N takes will naturally depend on the assumptions made concerning the $\tau_j(\vec{r}_j)$'s A case of interest arises when τ_j is the Gaussian distribution of $\vec{r}_j$

$$\tau_j = \frac{1}{(2\pi \ell_j^2/3)^{3/2}} \exp(-3|\vec{r}_j|^2/2\ell_j^2) \tag{A-23}$$

where ℓ_j^2 denotes the mean square displacement to be expected on the j-th occasion. While ℓ_j^2 may differ from one displacement to another, we assume that all the displacements occur in random directions.

For τ_j of the form.(A-23) our expression for $A_N(\vec{\rho})$ becomes

$$A_N(\vec{\rho}) = \prod_{j=1}^{N} \frac{1}{(2\pi\ell_j^2/3)^{3/2}} \iiint_{-\infty}^{\infty} \exp\left[i(\rho_1 x_j + \rho_2 y_j + \rho_3 z_j) - 3(x_j^2+y_j^2+z_j^2)/2\ell_j^2\right] \times dx_j\, dy_j\, dz_j$$

$$= \prod_{j=1}^{N} \exp\left[-(\rho_1^2+\rho_2^2+\rho_3^2)\ell_j^2/6\right] = \exp\left[-(|\vec{\rho}|^2 \sum_{j=1}^{N} \ell_j^2)/6\right] \tag{A-24}$$

where $\langle \ell^2 \rangle$ stand for

$$\langle \ell^2 \rangle = \frac{1}{N} \sum_{j=1}^{N} \ell_j^2 \tag{A-25}$$

From equation (A-24) and (A-25), $A_N(\vec{\rho})$ becomes

$$A_N(\vec{\rho}) = \exp\left[-N\langle \ell^2 \rangle |\vec{\rho}|^2/6\right] \tag{A-26}$$

Substituting for $A_N(\vec{\rho})$ in Eq.(A-21) we obtain

$$W_N(\vec{R}) = \frac{1}{8\pi^3} \iiint_{-\infty}^{\infty} \exp\left[-i(\rho_1 X + \rho_2 Y + \rho_3 Z) - N\langle \ell^2 \rangle(\rho_1^2+\rho_2^2+\rho_3^2)/6\right] \times d\rho_1\, d\rho_2\, d\rho_3 \tag{A-27}$$

The integrations in (A-27) are performed and we find

$$W_N(\vec{R}) = \frac{1}{(2\pi N\langle \ell^2 \rangle/3)^{3/2}} \exp\left[-3|\vec{R}|^2/2N\langle \ell^2 \rangle\right] \tag{A-28}$$

APPENDIX II

MULTIVARIATE GAUSSIAN DISTRIBUTIONS (6)

We considered the case of the problem of random flights in which the N displacements which the particle suffers are all governed by Gaussian dirtributions but with different variances. We shall now consider a generalization of this problem which has important applications to the theory of Brownian motion.

Let

$$\vec{\Psi} = \sum_{j=1}^{N} \psi_j \vec{r} \; ; \; \vec{\Phi} = \sum_{j=1}^{N} \phi_j \vec{r} \tag{A-29}$$

where the ψ_j's and the ϕ_j's are two arbitrary sets of N real numbers each, and where further $\vec{r}$ is a stochastic variable the probability distribution of which is governed by

$$\Upsilon(\vec{r}) = (1/(2\pi\ell^2)^{3/2}) \exp(-|\vec{r}|^2/2\ell^2) \tag{A-30}$$

where ℓ is a constant. We require the probablitily $W(\vec{\Psi},\vec{\Phi})\, d\vec{\Psi}\, d\vec{\Phi}$ that $\vec{\Psi}$ and $\vec{\Phi}$ shall lie, respectively, in the ranges $(\vec{\Psi}, \vec{\Psi} + d\vec{\Psi})$ and $(\vec{\Phi}, \vec{\Phi} + d\vec{\Phi})$. We have from Appendix I

$$W(\vec{\Psi},\vec{\Phi}) = \frac{1}{64\pi^6} \iint_{-\infty}^{\infty} \exp[-i(\vec{\rho}\cdot\vec{\Psi} + \vec{\sigma}\cdot\vec{\Phi})]\, A_N(\vec{\rho},\vec{\sigma})\, d\vec{\rho}\, d\vec{\sigma} \tag{A-31}$$

where $\vec{\rho}$ and $\vec{\sigma}$ are two auxiliary vectors and

$$A_N(\vec{\rho},\vec{\sigma}) = \prod_{j=1}^{N} \frac{1}{(2\pi\ell^2)} \int_{-\infty}^{\infty} \exp[i(\vec{\rho}\cdot\psi_j\vec{r} + \vec{\sigma}\cdot\phi_j\vec{r})] \times \exp(-|\vec{r}|^2/2\ell^2)\, d\vec{r} \tag{A-32}$$

To evaluate $A_N(\vec{\rho},\vec{\sigma})$ we need the value of the typical integral

$$J = \frac{1}{(2\pi\ell^2)^{3/2}}\int_{-\infty}^{\infty} exp[i\vec{r}\cdot(\psi_j\vec{\rho}+\phi_j\vec{\sigma}) - (|\vec{r}|^2/2\ell^2)]\,d\vec{r} \qquad (A-33)$$

We have

$$J = \prod_{x,y,z}\frac{1}{(2\pi\ell^2)^{3/2}}\int_{-\infty}^{\infty} exp\{-[x^2+2i\ell^2x(\rho_1\psi_j+\sigma_1\phi_j)]/2\ell^2\}\,dx \qquad (A-34)$$

$$= exp\{-\ell^2[(\rho_1\psi_j+\sigma_1\phi_j)^2+(\rho_2\psi_j+\sigma_2\phi_j)^2+(\rho_3\psi_j+\sigma_3\phi_j)^2]/2\}$$

Hence

$$A_N(\vec{\rho},\vec{\sigma}) = exp\{-\ell^2\sum_{j=1}^{N}[(\rho_1\psi_j+\sigma_1\phi_j)^2+(\rho_2\psi_j+\sigma_2\phi_j)^2 + (\rho_3\psi_j+\sigma_3\phi_j)^2]/2\} \qquad (A-35)$$

$$= exp[-P|\vec{\rho}|^2+2R\vec{\rho}\cdot\vec{\sigma}+Q|\vec{\sigma}|^2)/2]$$

where

$$P = \ell^2\sum_{j=1}^{N}\psi_j^2\ ,\quad R = \ell^2\sum_{j=1}^{N}\phi_j\psi_j\ ,\quad Q = \ell^2\sum_{j=1}^{N}\phi_j^2 \qquad (A-36)$$

Substituting for $A_N(\vec{\rho},\vec{\sigma})$ from Eq.(A-36) in $W(\vec{\Psi},\vec{\Phi})$ [Eq (A-31)] we obtain

$$W(\vec{\Psi},\vec{\Phi}) = \frac{1}{64\pi^6}\prod_{i=1}^{3}\iint_{-\infty}^{\infty} exp\{-[P\rho_i^2+2R\rho_i\sigma_i+Q\sigma_i^2+2i \times(\rho_i\Psi_i+\sigma_i\Phi_i)]/2\}\,d\rho_i\,d\sigma_i \qquad (A-37)$$

To evaluate the integrals occurring in the foregoing formula, we first perform a translation of the coordinate system according to

$$\rho_i = \xi_i+\alpha_i\ ,\quad \sigma_i = \eta_i+\beta_i \quad (i=1,2,3) \qquad (A-38)$$

where α_i and β_i are so chosen that

$$P\alpha_i+R\beta_i = -i\Psi_i\ ,\quad R\alpha_i+Q\beta_i = -i\Phi_i \quad (i=1,2,3) \qquad (A-39)$$

With this transformation of the variables we have

$$P\rho_i^2+2R\rho_i\sigma_i+Q\sigma_i^2+2i(\rho_i\Psi_i+\sigma_i\Phi_i) = P\xi_i^2+2R\xi_i\eta_i + Q\eta_i^2+i(\alpha_i\Psi_i+\beta_i\Phi_i) \qquad (A-40)$$

$$= P\xi_i^2 + 2R\xi_i\eta_i + Q\eta_i^2 + \frac{1}{(PQ-R^2)}(P\Phi_i^2 - 2R\Phi_i\Psi_i + Q\Psi_i^2)$$

Hence
$$W(\vec{\Psi},\vec{\Phi}) = \frac{1}{64\pi^6}\prod_{i=1}^{3} exp\left[-(P\Phi_i^2 - 2R\Phi_i\Psi_i + Q\Psi_i^2)\right. \qquad (A-41)$$

$$\left.\times 1/2(PQ-R^2)\right]\times\int\int_{-\infty}^{\infty} exp\left[-(P\xi_i^2 + 2R\xi_i\eta_i + Q\eta_i^2)/2\right] d\xi_i d\eta_i$$

From this equation we readily find that

$$W(\vec{\Psi},\vec{\Phi}) = \left[1/8\pi^3(PQ-R^2)^{3/2}\right] exp\left[-(P|\vec{\Phi}|^2 - 2R\vec{\Psi}.\vec{\Phi} + Q|\vec{\Psi}|^2)/2(PQ-R^2)\right] \qquad (A-42)$$

Which gives the required probability distribution.

APPENDIX III

CORRELATIONS IN A SYSTEM OF COUPLED CLASSICAL OSCILLATORS (10)

We will consider first the correlations of the initial values of the coordinates and momenta, whose the assumed distribution is canonical, i.e.,

$$D(\bar{q}(0), \bar{p}(0)) = (2\pi/\beta)^{2N+1} (\det \bar{A})^{-1/2}$$
$$\times \exp\left\{ -\frac{\beta}{2}\left[\sum_j p_j^2(0) + \sum_{j,k} q_j(0) A_{jk} q_k(0)\right]\right\} \qquad \text{(A-43)}$$

From this distribution, we obtain

$$\langle p_j(0) p_k(0)\rangle = kT\delta_{jk}$$
$$\langle p_j(0) q_k(0)\rangle = 0 \qquad \text{(A-44)}$$
$$\langle q_j(0) q_k(0)\rangle = kT\,||\bar{A}^{-1}||_{jk}$$

From the pair correlations for the time dependent coordinates and momenta obtained in Eq (5) of section-3.3 and (A-44), we have for the momentum correlation

$$\langle p_j(t)\, p_k(t+\tau)\rangle = \sum_{m,n}\Big\{||\bar{A}^{1/2}\sin\bar{A}^{1/2}t||_{jm}$$
$$\times\, ||\bar{A}^{1/2}\sin\bar{A}^{1/2}(t+\tau)||_{kn}\, \langle q_m(0) q_n(0)\rangle \qquad \text{(A-45)}$$
$$+\, ||\cos\bar{A}^{1/2}t||_{jm}\; ||\cos\bar{A}^{1/2}(t+\tau)||_{kn} \langle p_m(0) p_n(0)\rangle\Big\}$$
$$= kT\Big\{||\sin\bar{A}^{1/2}t\,\sin\bar{A}^{1/2}(t+\tau) + \cos\bar{A}^{1/2}t\,\cos\bar{A}^{1/2}(t+\tau)||_{jk}$$

From Eq (A-45), using the formula for the cosine of the differences of two values $\bar{A}^{1/2}t$ and $\bar{A}^{1/2}(t+\tau)$ and substituting the correlations of the initial values of the coordinats and momenta from Eq (A - 44), we have

$$\langle p_j(t)\, p_k(t+\tau)\rangle = kT \| \cos \bar{A}^{1/2} \tau \|_{jk} \qquad (A-46)$$

In a similar way, we get

$$\langle q_j(t)\, p_k(t+\tau)\rangle = -kT \| \bar{A}^{-1/2} \sin \bar{A}^{1/2} \tau \|_{jk} \qquad (A-47)$$

$$\langle q_j(t)\, q_k(t+\tau)\rangle = kT \| \bar{A}^{-1} \cos \bar{A}^{1/2} \tau \|_{jk} \qquad (A-48)$$

VITA

Name	Rachai Prakobkarn
Born	June 2, 1954.
Degree	B.Eng. (Civil), November, 1977.
	Chulalongkorn University
	Bangkok, Thailand.

หอสมุดกลาง สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย