Functional integrals in Brownian motion

1968 J. Phys. A: Gen. Phys. 1 431

(http://iopscience.iop.org/0022-3689/1/4/302)

J. PHYS. A (PROC. PHYS. SOC.), 1968, SER. 2, VOL. 1. PRINTED IN GREAT BRITAIN

Functional integrals in Brownian motion

G. J. PAPADOPOULOS
Department of Mathematics, University of Leeds
Communicated by S. F. Edwards; MS. received 21st February 1968

Abstract. The functional calculus is employed systematically for the development of the theory of Brownian motion. A simple method to obtain the Smoluchowski integral equation is devised. This equation forms the basis for the derivation of conditional functional integral representations over phase-space, momentum- and configuration-space functions of the phase-space conditional probability distribution. A functional steepest-descent method is employed for an approximate evaluation of the conditional probability distribution of the momenta.

1. Introduction

Particles in a liquid environment continuously suffer collisions, at random, from the molecules of the surrounding medium, due to the thermal agitation of the latter (Einstein 1956). As a result of the thermal kicks, a particle of approximately colloidal size is continuously executing an irregular random walk (kinks); we say that it executes Brownian motion or simply that it is a Brownian particle.

Langevin postulated the following equations of motion for the Brownian particle:

$$\frac{d\mathbf{p}}{d\tau} = -B\mathbf{p}+\mathbf{F}(\mathbf{r},\mathbf{p},\tau)+\mathbf{f}(\tau) \tag{1.1a}$$

$$\mathbf{p} = m\frac{d\mathbf{r}}{d\tau}. \tag{1.1b}$$

B^{-1} is a 3×3 relaxation time matrix, which is symmetric, positive definite and depends on the viscous properties of the medium and the geometry of the particle (see, e.g., Landau and Lifshitz (1959). The orientation dependence will be considered averaged. $-B\mathbf{p}$ is the Stokes resistance of the medium to the particle. $\mathbf{F}(\mathbf{r}, \mathbf{p}, \tau)$ is the external force on the particle, assumed to be slowly varying and containing no memory. $\mathbf{f}(\tau)$ is the force of collisions, assumed random and independent of the kinetic state of the particle. $\mathbf{f}(\tau)$ is also uncorrelated to its previous values. The linear dependence of the medium resistance on the particle momentum (Stokes law) is adequately correct for quasi-static motion. In general, the resistance contains a memory term. An example of this sort appears in Landau and Lifshitz (1959). However, the results based on the Stokes resistance show good agreement with experiment, as demonstrated by Perrin (1916). The forces $-B\mathbf{p}$ and $\mathbf{F}$ are called systematic, while the force $\mathbf{f}(\tau)$ is a thermal or collision force.

The motion of the Brownian particle cannot be studied deterministically owing to insufficient knowledge of the thermal force. Even if $\mathbf{f}(\tau)$ were known in detail, the rapidity and randomness of the kinks would render the task of following the particle motion impossible. Thus the need to recourse to a statistical treatment. What we need in this approach is the distribution of the thermal force. With the aid of this distribution we can obtain the distribution of the dynamic variables $\mathbf{r}, \mathbf{p}$, using their equations of motion (1.1*a*, *b*). Chandrasekhar (1943) assumed that in a short interval of time, in which a small change in $\mathbf{p}$ and $\mathbf{r}$ occurs, but a considerable number of collisions takes place, the probability distribution for $\mathbf{f}(\tau)$ is Gaussian. Owing to the independence of the thermal force on its previous history, the distribution of $\mathbf{f}$ in successive short time intervals is the product of the distributions for these intervals. With this distribution and the solutions of the equations of motion written in finite difference form as regards the part involving $\mathbf{f}(\tau)$, Chandrasekhar obtained the distribution of $\mathbf{r}, \mathbf{p}$ after letting the short time intervals go to zero. In actual fact, Chandrasekhar was using integration in the function space of the thermal force without explicitly stating it. The problems relevant to our work treated there were the case of the free Brownian particle (i.e. external force equal to zero) and the case of the harmonically bound particle. The friction coefficient mB was taken as a scalar and constant.

In this work we generalize and systematize Chandrasekhar's original method by integration in the function space of the thermal force. We proceed further to develop expressions for the distribution functions of $\mathbf{r}$, $\mathbf{p}$ as configuration-, momentum- and phase-space functional integrals. During the completion of this work, we found that Onsager and Machlup (1953) obtained similar expressions for particular cases. Reference will be made to these cases later in the text.

The problem we treat here is: given a functional distribution for the thermal force $\mathbf{f}(\tau)$ over a time interval $[t', t)$, we require the distribution for the position $\mathbf{r}$ and momentum $\mathbf{p}$ of the particle at time t, given that at an earlier time t' the particle occupied the phase point $(\mathbf{r}', \mathbf{p}')$. We make the stochastic assumption that the functional distribution of the thermal force over $[t', t)$ is the following continual Gaussian distribution:

$$W[\mathbf{f}_{t'}{}^{t}(\tau)] = \left[\prod_{t' \leqslant \tau < t} \det\{\pi^{-1} g(\tau)\, d\tau\}\right]^{1/2} \exp\left\{-\int_{t'}^{t} g_{\alpha\beta}(\tau) f_{\alpha}(\tau) f_{\beta}(\tau)\, d\tau\right\}. \tag{1.2}$$

The summation convention from 1 to 3 will be assumed for repeated indices throughout this text. g is a positive definite symmetric matrix. It can be further specified so that, for a free Brownian particle (i.e. $\mathbf{F} = 0$), the distribution of the momentum after infinite time goes over to the Maxwellian distribution:

$$(2\pi m\kappa T)^{-3/2} \exp\left(-\frac{\mathbf{p}^2}{2m\kappa T}\right). \tag{1.3}$$

Alternatively, we demand that the equation governing the distribution of the particle momentum admits (1.3) as a solution in the case $\mathbf{F} = 0$. The matrix $\mathbf{g}$, thus determined, is

$$g^{-1} = 4\kappa TmB. \tag{1.4}$$

This was done in an earlier work by the author (Papadopoulos 1967, to be referred to as I).

One may consider the functional distribution (1.2) as the distribution of the collision forces $\mathbf{f}(\tau)$ acting on the particles of an ensemble of identical Brownian particles, for all $\tau \in [t', t)$. It is easy to deduce that the thermal forces at two different times are not correlated. This fact, together with the non-existence of memory terms in the equations of motion for $\mathbf{r}$ and $\mathbf{p}$ secure the Markovicity of these variables.

The statistical description of the Brownian motion is effected through the ensemble average conditional probability distribution (ECPD) $G(\mathbf{p}|\mathbf{p}', \mathbf{r}|\mathbf{r}'; t|t')$, $t > t'$, of finding the particle in the vicinity of the phase point $(\mathbf{r}, \mathbf{p})$ at time t, if at an earlier time t' it occupied the phase point $(\mathbf{r}', \mathbf{p}')$. It is our object in the subsequent sections to develop techniques for obtaining the ECPD.

In § 2 following Edwards (1964) we obtain the ECPD G as a functional average of the corresponding conditional probability distribution (CPD) in the deterministic (or Liouville) sense. The method is exemplified by (*a*) calculating the ECPD when the external force is a prescribed function of time and (*b*) by finding the same distribution in the general case, when the external force $\mathbf{F} = \mathbf{F}(\mathbf{p}, \mathbf{r}, \tau)$, but for $t - t'$ very short.

In § 3, exploiting the method for the construction of the ECPD G, we devise a simple method to show that G obeys the Kolmogorov–Chapman (or otherwise Smoluchowski) integral equation. This property is usually assumed. Also we show that G is a Green function of the Fokker–Planck equation.

Section 4 deals with formal representations of G as conditional functional integrals in momentum, configuration and phase spaces.

Finally, in § 5, we deal with an approximation method analogous to the WKB approximation. Considering the case where $\mathbf{F} = \mathbf{F}(\mathbf{p}, \tau)$ and employing the functional integral expressions over momentum functions, we obtain a compact approximate expression for the ECPD of the momentum. In the case where the external force is a function of time and linearly dependent on the momentum, the method yields exact results. Onsager and Machlup used this method with zero external force and obtained an exact expression for the exponential factor of the probability. In the general case of $\mathbf{F}(\mathbf{p}, \mathbf{r}, \tau)$ the complete expression obtained by this method involves another factor dependent on $\mathbf{r}$, $\mathbf{p}$. We have calculated this factor in the case $\mathbf{F} = \mathbf{F}(\mathbf{p}, \tau)$. We believe that this calculation demonstrates the power of functional techniques to reach results, which otherwise are difficult of access.

2. Construction of the ECPD $G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t')$

In I under certain restrictions we introduced the method for the construction of the ECPD in momentum space. We wish now to extend the construction in phase space. Let

$$\mathbf{R}(t) = \mathbf{R}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)]), \qquad \mathbf{P}(t) = \mathbf{P}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)]) \tag{2.1}$$

be the solution of equations (1.1a, b), which satisfy the initial condition

$$\mathbf{R}(t') = \mathbf{r}', \qquad \mathbf{P}(t') = \mathbf{p}'. \tag{2.2}$$

The deterministic CPD of finding the particle in the vicinity of the phase point $(\mathbf{r}, \mathbf{p})$ at time t, if at an earlier time t' the particle occupied the phase point $(\mathbf{r}', \mathbf{p}')$ is given by

$$\delta\{\mathbf{r}-\mathbf{R}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)])\} \times \delta\{\mathbf{p}-\mathbf{P}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)])\}. \tag{2.3}$$

The ECPD is obtained as the functional average of the deterministic CPD over the functional thermal force distribution. We have

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = \int \delta\{\mathbf{r}-\mathbf{R}(t)\}\delta\{\mathbf{p}-\mathbf{P}(t)\} W[\mathbf{f}_{t'}{}^{t}(\tau)] \prod_{t' \leqslant \tau < t} d\mathbf{f}(\tau). \tag{2.4}$$

In the following, we shall give a few explicit calculations of G using formula (2.4). We shall make use of the following functional integration formula:

$$\int \delta\left\{\mathbf{X}^{(1)} - \int_{t'}^{t} Q^{(1)}(\tau)\mathbf{f}(\tau)\,d\tau\right\} \delta\left\{\mathbf{X}^{(2)} - \int_{t'}^{t} Q^{(2)}(\tau)\mathbf{f}(\tau)\,d\tau\right\} W[\mathbf{f}_{t'}{}^{t}(\tau)] \prod_{t' \leqslant \tau < t} d\mathbf{f}(\tau)$$

$$= \left[\det\left\{\pi \int_{t'}^{t} K(\tau)\,d\tau\right\}\right]^{-1/2} \exp\left[-\sum_{r,s=1}^{2\times 3} \left\{\int_{t'}^{t} K(\tau)\,d\tau\right\}_{rs}^{-1} X_r{}'X_s{}'\right] \tag{2.5}$$

where $\mathbf{X}^{(1)}$, $\mathbf{X}^{(2)}$ are three-dimensional vectors and $\underset{\sim}{Q}^{(1)}$, $\underset{\sim}{Q}^{(2)}$ are 3×3 matrices. K is the 6×6 matrix given in partitioned form (see appendix of I):

$$K(\tau) = \begin{bmatrix} Q^{(1)}g^{-1}\tilde{Q}^{(1)} & Q^{(1)}g^{-1}\tilde{Q}^{(2)} \\ Q^{(2)}g^{-1}\tilde{Q}^{(1)} & Q^{(2)}g^{-1}\tilde{Q}^{(2)} \end{bmatrix} \tag{2.5a}$$

and

$$X_1{}' = X_1{}^{(1)}, \quad X_2{}' = X_2{}^{(1)}, \quad X_3{}' = X_3{}^{(1)}, \quad X_4{}' = X_1{}^{(2)}, \quad X_5{}' = X_2{}^{(2)}, \quad X_6{}' = X_3{}^{(2)}$$

$\tilde{Q}^{(j)}$ stands for the transpose of $Q^{(j)}$.

(i) As a first example, we consider a Brownian particle under the influence of a time-prescribed force $\mathbf{F}(\tau)$. We shall also take the relaxation time matrix B constant, as this is the usual case in applications. In this case the Langevin equations are

$$\begin{aligned} \frac{d\mathbf{p}}{d\tau} &= -B\mathbf{p} + \mathbf{F}(\tau) + \mathbf{f}(\tau) \\ \mathbf{p} &= m\frac{d\mathbf{r}}{d\tau}. \end{aligned} \tag{2.6}$$

The solution of (2.6) satisfying $\mathbf{R}(t') = \mathbf{r}'$, $\mathbf{P}(t') = \mathbf{p}'$ is given by

$$\begin{aligned} \mathbf{R}(t) &= \mathbf{V} + \int_{t'}^{t} m^{-1}B^{-1}[I - \exp\{-B(t-\tau)\}]\mathbf{f}(\tau)\,d\tau \\ \mathbf{P}(t) &= \mathbf{v} + \int_{t'}^{t} \exp\{-B(t-\tau)\}\mathbf{f}(\tau)\,d\tau \end{aligned} \tag{2.7a}$$

where

$$\begin{aligned} \mathbf{V} &= \mathbf{r}' + m^{-1}B^{-1}[I - \exp\{-B(t-t')\}]\mathbf{p}' + m^{-1}B^{-1}\int_{t'}^{t}[I - \exp\{-B(t-\tau)\}]\mathbf{F}(\tau)\,d\tau \\ \mathbf{v} &= \exp\{-B(t-t')\}\mathbf{p}' + \int_{t'}^{t} \exp\{-B(t-\tau)\}\mathbf{F}(\tau)\,d\tau. \end{aligned} \tag{2.7b}$$

I stands for the 3×3 unit matrix. Employing formula (2.4), we obtain for the ECPD in phase space the result

$$\begin{aligned} G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') &= \int \delta\left(\mathbf{r} - \mathbf{V} - \int_{t'}^{t} m^{-1}B^{-1}[I - \exp\{-B(t-\tau)\}]\mathbf{f}(\tau)\,d\tau\right) \\ &\quad \times \delta\left[\mathbf{p} - \mathbf{v} - \int_{t'}^{t} \exp\{-B(t-\tau)\}\mathbf{f}(\tau)\,d\tau\right] W[\mathbf{f}_{t'}^{\,t}(\tau)] \prod_{t' \leqslant \tau < t} d\mathbf{f}(\tau) \\ &= \left[\det\left\{\pi\begin{pmatrix} A^{(1)} & A^{(2)} \\ A^{(2)} & A^{(3)} \end{pmatrix}\right\}\right]^{-1/2} \exp\left\{-\sum_{\alpha,\beta=1}^{6} \begin{pmatrix} A^{(1)} & A^{(2)} \\ A^{(2)} & A^{(3)} \end{pmatrix}^{-1}_{\alpha\beta} y_\alpha y_\beta\right\} \end{aligned} \tag{2.8}$$

where

$$\begin{aligned} A^{(1)} &= 4\kappa T m^{-1}B^{-1}[(t-t') - \tfrac{3}{2}B^{-1} + 2B^{-1}\exp\{-B(t-t')\} - \tfrac{1}{2}B^{-1}\exp\{-2B(t-t')\}] \\ A^{(2)} &= 4\kappa T B^{-1}[\tfrac{1}{2} - \exp\{-B(t-t')\} + \tfrac{1}{2}\exp\{-2B(t-t')\}] \\ A^{(3)} &= 4\kappa T m[\tfrac{1}{2} - \tfrac{1}{2}\exp\{-2B(t-t')\}]. \end{aligned} \tag{2.8a}$$

Since B is symmetric and the matrices $A^{(1)}$, $A^{(2)}$ and $A^{(3)}$ can be analysed in power series of B, it follows that these matrices are also symmetric. Furthermore, they commute. $\mathbf{y}$ is a six-dimensional phase vector with components

$$y_\alpha = r_\alpha - V_\alpha \ (\alpha = 1, 2, 3) \quad \text{and} \quad y_{3+j} = p_j - v_j \ (j = 1, 2, 3). \tag{2.8b}$$

We have made use of the relation $g^{-1} = 4\kappa T m B$. Formula (2.8) as it stands is not convenient for calculations. It is possible to express the determinant and the inverse of the 6×6 partitioned matrix involved in a convenient manner. We observe that

$$\begin{pmatrix} A^{(1)} & A^{(2)} \\ A^{(2)} & A^{(3)} \end{pmatrix}\begin{pmatrix} A^{(3)} & -A^{(2)} \\ -A^{(2)} & A^{(1)} \end{pmatrix} = \begin{pmatrix} A^{(1)}A^{(3)} - (A^{(2)})^2 & 0 \\ 0 & A^{(1)}A^{(3)} - (A^{(2)})^2 \end{pmatrix} \tag{2.9}$$

where we have used the commutativity of the matrices $A^{(j)}$ $(j = 1, 2, 3)$. From (2.9) we obtain

$$\begin{pmatrix} A^{(1)} & A^{(2)} \\ A^{(2)} & A^{(3)} \end{pmatrix}^{-1} = \begin{pmatrix} A^{(3)}\{A^{(1)}A^{(3)} - (A^{(2)})^2\}^{-1}, & -A^{(2)}\{A^{(1)}A^{(3)} - (A^{(2)})^2\}^{-1} \\ -A^{(2)}\{A^{(1)}A^{(3)} - (A^{(2)})^2\}^{-1}, & A^{(1)}\{A^{(1)}A^{(3)} - (A^{(2)})^2\}^{-1} \end{pmatrix}. \tag{2.9a}$$

In (2.9a) we have managed to express the inverse of the 6×6 partitioned matrix on the left-hand side in terms of the inverse of the 3×3 matrix $A^{(1)}A^{(3)} - (A^{(2)})^2$. From (2.8$a$) we have

$$\begin{aligned} A^{(1)}A^{(3)} - (A^{(2)})^2 &= (4\kappa T)^2 B^{-1}[\tfrac{1}{2}(t-t') + 2B^{-1}\exp\{-B(t-t')\} \\ &\quad - \{\tfrac{3}{4}B^{-1} + \tfrac{1}{2}(t-t')\}\exp\{-2B(t-t')\}]. \end{aligned} \tag{2.9b}$$

The 3×3 matrices on the right-hand side of (2.9*a*) are functions of the matrix B. Let us introduce the notation

$$\varphi^{(j)}(B) = A^{(j)}(B)[A^{(1)}(B)A^{(3)}(B) - \{A^{(2)}(B)\}^2]^{-1}. \tag{2.9c}$$

If we let S be a similarity matrix corresponding to B, i.e.

$$SBS^{-1} = D \tag{2.9d}$$

where D is a diagonal matrix (its diagonal elements being the eigenvalues of B in some order), we have

$$\varphi^{(j)}(B) = S^{-1}S\varphi^{(j)}(B)S^{-1}S = S^{-1}\varphi^{(j)}(D)S. \tag{2.9e}$$

$\varphi^{(j)}(D)$ is diagonal and therefore the inversion involved in (2.9*c*) is quite simple, and we shall not pursue the calculation of the φ's any more. From (2.9), by observing that the determinants of each of the matrices on the left-hand side are equal, we find that

$$\det\begin{pmatrix} A^{(1)} & A^{(2)} \\ A^{(2)} & A^{(3)} \end{pmatrix} = \det[A^{(1)}(D)A^{(3)}(D) - \{A^{(2)}(D)\}^2]. \tag{2.9f}$$

The right-hand side of (2.9*f*) is easily calculable once the eigenvalues of the matrix B are known. Now from (2.8) and (2.9*a*, *c*, *e*, *f*) we find for the ECPD the result

$$\begin{aligned} G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = {} & \{\det(\pi^2[A^{(1)}(D)A^{(3)}(D) - \{A^{(2)}(D)\}^2])\}^{-1/2} \\ & \times \exp[-\{\varphi^{(1)}(B)\}_{\alpha\beta}(r_\alpha - V_\alpha)(r_\beta - V_\beta) - 2\{\varphi^{(2)}(B)\}_{\alpha\beta}(r_\alpha - V_\alpha)(p_\beta - v_\beta) \\ & - \{\varphi^{(3)}(B)\}_{\alpha\beta}(p_\alpha - v_\alpha)(p_\beta - v_\beta)]. \end{aligned} \tag{2.10}$$

Formula (2.10) is a generalization of a result due to Chandrasekhar (1943) for the free Brownian particle with scalar relaxation time. Our formula takes account of a time-prescribed systematic force and matrix relaxation time. We shall not dwell here on the asymptotic form taken by (2.10) for $t - t' \gg B^{-1}$.

(ii) We now wish to find the ECPD $G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t+\Delta t|t)$ of finding the particle at time $t+\Delta t$ in the vicinity of the phase point $(\mathbf{r}, \mathbf{p})$ given that at an earlier time t the particle occupied the phase point $(\mathbf{r}', \mathbf{p}')$. The time Δt is taken short enough so that the systematic forces do not change appreciably. However, the collision force in this time interval undergoes large variations.

From the Langevin equations (1.1*a*, *b*) we obtain for

$$\mathbf{R}(t) = \mathbf{r}' \quad \text{and} \quad \mathbf{P}(t) = \mathbf{p}'$$

$$\mathbf{R}(t+\Delta t) = \mathbf{r}' + m^{-1}\int_t^{t+\Delta t} \mathbf{p}(\tau)\,d\tau \simeq \mathbf{r}' + m^{-1}\mathbf{p}'\Delta t \tag{2.11a}$$

$$\begin{aligned} \mathbf{P}(t+\Delta t) &= \mathbf{p}' + \int_t^{t+\Delta t} [-B\mathbf{p}(\tau) + \mathbf{F}\{\mathbf{r}(\tau), \mathbf{p}(\tau), \tau\}]\,d\tau + \int_t^{t+\Delta t} \mathbf{f}(\tau)\,d\tau \\ &= \mathbf{p}' + \{-B\mathbf{p} + \mathbf{F}(\mathbf{r}', \mathbf{p}', t)\}\Delta t + \int_t^{t+\Delta t} \mathbf{f}(\tau)\,d\tau \end{aligned} \tag{2.11b}$$

where we have replaced the time integral of the systematic forces by the first non-vanishing term of its Taylor expansion. This is done on account of the small variation of the systematic forces. We cannot do this for the thermal force owing to its rapid variation. We remark that for short-time intervals the displacement of the Brownian particle does not depend explicitly on the collision force.

Employing (2.4) for the construction of the ECPD we have

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t+\Delta t|t) = \delta\{\mathbf{r} - \mathbf{R}(t+\Delta t)\}\int \delta\{\mathbf{p} - \mathbf{P}(t+\Delta t)\}W[\mathbf{f}_{t'}{}^{t}(\tau)] \prod_{t \leqslant \tau < t+\Delta t} d\mathbf{f}(\tau). \tag{2.12}$$

The functional integral in (2.12) is given by (II.9) in I if one replaces $\mathbf{F}(\mathbf{p}', t)$ by $\mathbf{F}(\mathbf{r}', \mathbf{p}', t)$ since the presence of $\mathbf{r}'$ in $\mathbf{F}$ does not affect the functional dependence of $\mathbf{P}(t+\Delta t)$ on $\mathbf{f}(\tau)$. We have

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = \delta\{\mathbf{r}-\mathbf{r}'-m^{-1}\mathbf{p}'\Delta t\}[\det\{\pi g^{-1}(t)\Delta t\}]^{-1/2}$$
$$\times \exp\left\{-g_{\alpha\beta}(t)\left(\frac{\mathbf{p}-\mathbf{p}'}{\Delta t}+B(t)\mathbf{p}'-\mathbf{F}(\mathbf{r}', \mathbf{p}', t)\right)_\alpha\right.$$
$$\left.\times\left(\frac{\mathbf{p}-\mathbf{p}'}{\Delta t}+B(t)\mathbf{p}'-\mathbf{F}(\mathbf{r}', \mathbf{p}', t)\right)_\beta \Delta t\right\} \tag{2.13}$$

introducing the transformation

$$\mathbf{r}' = \mathbf{r}-\Delta\mathbf{r}', \qquad \mathbf{p}' = \mathbf{p}-\Delta\mathbf{p}'. \tag{2.14}$$

Formula (2.13) takes the form of a function $T(\mathbf{r}-\Delta\mathbf{r}', \mathbf{p}-\Delta\mathbf{p}'; \Delta\mathbf{r}', \Delta\mathbf{p}')$ and represents the transition probability density for the particle occupying the phase point $(\mathbf{r}-\Delta\mathbf{r}', \mathbf{p}-\Delta\mathbf{p}')$ at time t to change phase position by $(\Delta\mathbf{r}', \Delta\mathbf{p}')$ in the short time Δt. For later reference, we shall find the transition probability distribution for the particle to move from the phase point $(\mathbf{r}, \mathbf{p})$ at time t to $(\Delta\mathbf{r}, \Delta\mathbf{p})$ in the short time Δt. This is readily obtained from (2.13) as

$$T(\mathbf{r}, \mathbf{p}; \Delta\mathbf{r}, \Delta\mathbf{p}) = \delta\{\Delta\mathbf{r}-m^{-1}\mathbf{p}\Delta t\}[\det\{\pi g^{-1}(t)\Delta t\}]^{-1/2}$$
$$\times \exp\left\{-g_{\alpha\beta}(t)\left(\frac{\Delta\mathbf{p}}{\Delta t}+B\mathbf{p}-\mathbf{F}(\mathbf{r}, \mathbf{p}, t)\right)_\alpha\left(\frac{\Delta\mathbf{p}}{\Delta t}+B\mathbf{p}-\mathbf{F}(\mathbf{r}, \mathbf{p}, t)\right)_\beta \Delta t\right\}. \tag{2.15}$$

The following averages defined by

$$\langle\psi(\Delta\mathbf{r}, \Delta\mathbf{p})\rangle = \int \psi(\Delta\mathbf{r}, \Delta\mathbf{p})T(\mathbf{r}, \mathbf{p}; \Delta\mathbf{r}, \Delta\mathbf{p})\, d(\Delta\mathbf{r})\, d(\Delta\mathbf{p}) \tag{2.16}$$

will be utilized later on:

$$\begin{aligned}
\langle 1\rangle &= 1 \\
\langle\Delta r_\alpha\rangle &= m^{-1}p_\alpha\Delta t, \qquad \Delta p_\alpha = \{F_\alpha(\mathbf{r}, \mathbf{p}, t)-(B\mathbf{p})_\alpha\}\Delta t \\
\langle\Delta p_\alpha\Delta p_\beta\rangle &= \tfrac{1}{2}(g^{-1})_{\alpha\beta}\Delta t \\
\langle\Delta r_\alpha\Delta r_\beta\rangle, \langle\Delta r_\alpha\Delta p_\beta\rangle, &\langle\Delta p_\alpha\Delta p_\beta\Delta p_\gamma\rangle, \ldots \quad \text{are} \quad O((\Delta t)^2).
\end{aligned} \tag{2.17}$$

3. The Smoluchowski and Fokker–Planck equations

We wish to show that the ECPD defined in (2.4) obeys the Smoluchowski (Kolmogorov–Chapman) integral equation, i.e. for $t' < t_1 < t$,

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = \int G(\mathbf{r}|\mathbf{r}_1, \mathbf{p}|\mathbf{p}_1; t|t_1)G(\mathbf{r}_1|\mathbf{r}', \mathbf{p}_1|\mathbf{p}'; t_1|t)\, d\mathbf{r}_1\, d\mathbf{p}_1. \tag{3.1}$$

Proof. Since the equations of motion (1.1*a*, *b*) have no memory, it follows that for $t' < t_1 < t$ we have

$$\begin{aligned}
\mathbf{R}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)]) &= \mathbf{R}(\mathbf{R}_1, \mathbf{P}_1, [\mathbf{f}_{t_1}{}^{t}(\tau)]) \\
\mathbf{P}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t}(\tau)]) &= \mathbf{P}(\mathbf{R}_1, \mathbf{P}_1, [\mathbf{f}_{t_1}{}^{t}(\tau)])
\end{aligned} \tag{3.2}$$

where

$$\mathbf{R}_1 = \mathbf{R}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t_1}(\tau)]), \qquad \mathbf{P}_1 = \mathbf{P}(\mathbf{r}', \mathbf{p}', [\mathbf{f}_{t'}{}^{t_1}(\tau)]). \tag{3.2a}$$

Using (3.2) we verify that

$$\begin{aligned}\delta\{\mathbf{r}-\mathbf{R}(\mathbf{r}',\mathbf{p}',[\mathbf{f}_{t'}{}^{t}(\tau)])\}\delta\{\mathbf{p}-\mathbf{P}(\mathbf{r}',\mathbf{p}',[\mathbf{f}_{t'}{}^{t}(\tau)])\}\\ = \int \delta\{\mathbf{r}-\mathbf{R}(\mathbf{r}_1,\mathbf{p}_1,[\mathbf{f}_{t_1}{}^{t}(\tau)])\}\delta\{\mathbf{p}-\mathbf{P}(\mathbf{r}_1,\mathbf{p}_1,[\mathbf{f}_{t_1}{}^{t}(\tau)])\}\\ \times\delta\{\mathbf{r}_1-\mathbf{R}(\mathbf{r}',\mathbf{p}',[\mathbf{f}_{t'}{}^{t_1}(\tau)])\}\delta\{\mathbf{p}_1-\mathbf{P}(\mathbf{r}',\mathbf{p}',[\mathbf{f}_{t'}{}^{t_1}(\tau)])\}\,d\mathbf{t}_1\,d\mathbf{p}_1.\end{aligned} \quad (3.3)$$

The thermal distribution (1.3) factorizes for any pair of disjoint subintervals covering $[t', t]$, i.e.

$$W[\mathbf{f}_{t'}{}^{t}(\tau)] = W[\mathbf{f}_{t'}{}^{t_1}(\tau)]\,.\,W[\mathbf{f}_{t_1}{}^{t}(\tau)]. \quad (3.4)$$

Multiplying (3.3) and (3.4) by members and integrating both sides over all $\mathbf{f}(\tau)$, $\tau\epsilon[t', t]$ we obtain, using (2.4) for the ECPD, the Smoluchowski integral equation (3.1). It must be noted that, if the Langevin equations of motion contain memory or the thermal distribution does not factorize, then the Smoluchowski integral equation does not apply.

The Smoluchowski integral equation forms the basis for all calculations of Brownian motion. We shall derive from this equation for the ECPD—the Fokker–Planck equation. Let us replace t_1 by t and t by $t+\Delta t$ in (3.1) and introduce the transformation (2.14). Then using (2.13) we obtain

$$\begin{aligned}G(\mathbf{r}|\mathbf{r}',\mathbf{p}|\mathbf{p}';t+\Delta t|t') = T(\mathbf{r}-\Delta\mathbf{r},\mathbf{p}-\Delta\mathbf{p};\Delta\mathbf{r},\Delta\mathbf{p})\\ \times G(\mathbf{r}-\Delta\mathbf{r}|\mathbf{r}',\mathbf{p}-\Delta\mathbf{p}|\mathbf{p}';t|t')\,d(\Delta\mathbf{r})\,d(\Delta\mathbf{p}).\end{aligned} \quad (3.5)$$

The Fokker–Planck equation for the probability distribution $\Phi(\mathbf{r},\mathbf{p};t)$ is obtained from the same integral equation (3.5), i.e.

$$\Phi(\mathbf{r},\mathbf{p};t+\Delta t) = \int T(\mathbf{r}-\Delta\mathbf{r},\mathbf{p}-\Delta\mathbf{p};\Delta\mathbf{r},\Delta\mathbf{p})\Phi(\mathbf{r}-\Delta\mathbf{r},\mathbf{p}-\Delta\mathbf{p};t)\,d(\Delta\mathbf{r})\,d(\Delta\mathbf{p}) \quad (3.5a)$$

(see e.g. Chandrasekhar 1943). Expanding the left-hand side of (3.5*a*) in power series of Δt and the right-hand side in power series of Δr_α, Δp_α by Taylor's theorem and making some rearrangements, we have

$$\begin{aligned}\Phi+\frac{\partial\Phi}{\partial t}\Delta t+\mathrm{O}((\Delta t)^2) = \int\Big(\Phi T-\frac{\partial}{\partial r_\alpha}\Phi T\Delta r_\alpha-\frac{\partial}{\partial p_\alpha}\Phi T\Delta p_\alpha+\frac{1}{2}\frac{\partial^2}{\partial r_\alpha\partial r_\beta}\Phi T\Delta r_\alpha\Delta r_\beta\\ +\frac{\partial^2}{\partial r_\alpha\partial p_\beta}\Phi T\Delta r_\alpha\Delta p_\beta+\frac{1}{2}\frac{\partial^2}{\partial p_\alpha\partial p_\beta}\Phi\Delta p_\alpha\Delta p_\beta+\ldots\Big)\,d(\Delta\mathbf{r})\,d(\Delta\mathbf{p})\end{aligned} \quad (3.6)$$

where Φ and T denote the functions $\Phi(\mathbf{r},\mathbf{p};t)$ and $T(\mathbf{r},\mathbf{p};\Delta\mathbf{r},\Delta\mathbf{p})$. Using in (3.6) the averages obtained in (2.17), dividing both sides by Δt and passing to the limit as $\Delta t\to 0$, we obtain the partial differential equation

$$\left\{\frac{\partial}{\partial t}+\frac{\partial}{\partial r_\alpha}m^{-1}p_\alpha+\frac{\partial}{\partial p_\alpha}F_\alpha(\mathbf{r},\mathbf{p},t)\right\}\Phi = \left\{\frac{\partial}{\partial p_\alpha}(Bp_\alpha)+\frac{1}{4}\frac{\partial^2}{\partial p_\alpha\partial p_\beta}(g^{-1})_{\alpha\beta}\right\}\Phi. \quad (3.7)$$

This is the Fokker–Planck equation in phase space. In I we established for g the expression $g^{-1} = 4\kappa TmB$. By considering the case where the friction matrix $m^{-1}B$ is zero (i.e. when the particle does not dissipate energy to the environment) the resulting equation is Liouville's equation. The Fokker–Planck equation is a generalization of Liouville's equation to include dissipation phenomena.

Since for $t > t'$ the ECPD G satisfies (3.5*a*), it follows that, for $t > t'$, G defined in (2.4) is a solution of the Fokker–Planck equation (3.7). Furthermore, from (2.13) it is easy to see that as $\Delta t\to 0$ (changing t to t' and $t+\Delta t$ to t)

$$\begin{aligned}G(\mathbf{r}|\mathbf{r}',\mathbf{p}|\mathbf{p}';t|t')\to\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{p}-\mathbf{p}')\\ \text{as}\quad t\to t'+0.\end{aligned} \quad (3.8)$$

Since G satisfies the Fokker–Planck equation and property (3.8), it follows that it is a Green function of the Fokker–Planck equation. Furthermore, G has the property to propagate the solutions of the Fokker–Planck equation in phase space. In other words, if $\Phi(\mathbf{r}, \mathbf{p}; t')$ is the phase distribution at time t', the distribution $\Phi(\mathbf{r}, \mathbf{p}; t)$ at a later time $t > t'$, which obeys the Fokker–Planck equation and the same boundary conditions with respect to $\mathbf{r}$, $\mathbf{p}$ as G, is given by

$$\Phi(\mathbf{r}, \mathbf{p}; t) = \int G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t')\Phi(\mathbf{r}', \mathbf{p}'; t')\, d\mathbf{r}'\, d\mathbf{p}'. \tag{3.9}$$

This is the propagation equation. Φ in (3.9) satisfies the Fokker–Planck equation since G with respect to $\mathbf{r}, \mathbf{p}; t$ does so. The same applies for the boundary conditions. The initial condition requirement follows from (3.8) since

$$\Phi(\mathbf{r}, \mathbf{p}; t) \to \int \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{p}-\mathbf{p}')\Phi(\mathbf{r}', \mathbf{p}'; t')\, d\mathbf{r}'\, d\mathbf{p}' = \Phi(\mathbf{r}, \mathbf{p}; t') \tag{3.10}$$

$$\text{as} \quad t \to t'+0.$$

4. The ECPD $G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t')$ as a conditional functional integral

In I we produced a conditional functional integral over momentum-space functions for the Green function $G(\mathbf{p}|\mathbf{p}'; t|t')$. We wish now to consider the general case of the phase-space conditional probability distribution $G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t')$ as a conditional functional integral over α, phase-space functions, β, momentum-space functions and γ, configuration-space functions.

Let us at first consider a fine subdivision of the interval $[t', t]$:

$$\mathscr{D}_N = \{t_0, t_1, t_2, \ldots, t_N\}$$

with

$$t_0 = t' < t_1 < t_2 < \ldots < t_N = t.$$

We define $\Delta t_j = t_{j+1} - t_j$. Repeated application of Smoluchowski's integral equation (3.1) gives

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = \int G(\mathbf{r}|\mathbf{r}_{N-1}, \mathbf{p}|\mathbf{p}_{N-1}; t|t_{N-1})G(\mathbf{r}_{N-1}|\mathbf{r}_{N-2}, \mathbf{p}_{N-1}|\mathbf{p}_{N-2}; t_{N-1}|t_{N-2}) \ldots$$
$$\times G(r_2|r_1, p_2|p_1; t_2|t_1)G(\mathbf{r}_1|\mathbf{r}', \mathbf{p}_1|\mathbf{p}'; t_1|t')\, d\mathbf{r}_{N-1}\, d\mathbf{p}_{N-1} \ldots d\mathbf{t}_1\, d\mathbf{p}_1. \tag{4.1}$$

If we employ formula (2.13) for the ECPD between two neighbouring times,

$$G(\mathbf{r}_{j+1}|\mathbf{r}_j, \mathbf{p}_{j+1}|\mathbf{p}_j; t_{j+1}|t_j) \simeq \delta(\mathbf{r}_{j+1} - \mathbf{r}_j - m^{-1}\mathbf{p}_j\Delta t_j)\,.\,[\det\{\pi g^{-1}(t_j)\Delta t_j\}]^{-1/2}$$
$$\times \exp\left\{-g_{\alpha\beta}(t_j)\left(\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j} + B(t_j)\mathbf{p}_j - \mathbf{F}(\mathbf{r}_j, \mathbf{p}_j, t_j)\right)_\alpha\right.$$
$$\left.\times \left(\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j} + B(t_j)\mathbf{p}_j - \mathbf{F}(\mathbf{r}_j, \mathbf{p}_j, t_j)\right)_\beta \Delta t_j\right\}. \tag{4.2}$$

This gives the probability distribution for the Brownian particle starting from the phase point $(\mathbf{r}_j, \mathbf{p}_j)$ at time t_j to find itself in the vicinity of the phase point $(\mathbf{r}_{j+1}, \mathbf{p}_{j+1})$ at a neighbouring later time t_{j+1}. Substituting (4.2) into (4.1), repeatedly, we obtain for the ECPD

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') \simeq G^{(N)}(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t')$$
$$= \int \left[\prod_{j=0}^{N-1} \det\{\pi g^{-1}(t_j)\Delta t_j\}\right]^{-1/2}$$
$$\times \exp\left\{-\sum_{j=0}^{N-1} g_{\alpha\beta}(t_j)\left(\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j} + B(t_j)\mathbf{p}_j - \mathbf{F}(\mathbf{r}_j, \mathbf{p}_j, t_j)\right)_\alpha\right.$$

$$\times \left(\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j}+B(t_j)\mathbf{p}_j-\mathbf{F}(\mathbf{r}_j,\mathbf{p}_j,t_j)\right)_\beta \Delta t_j\Big\}$$
$$\times\left\{\prod_{j=0}^{N-1}\delta\left(\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}-m^{-1}\mathbf{p}_j\right)(\Delta t_j)^3\right\}\delta(\mathbf{r}_0-\mathbf{r}')\delta(\mathbf{p}_0-\mathbf{p}')$$
$$\times\delta(\mathbf{r}_N-\mathbf{r})\delta(\mathbf{p}_N-\mathbf{p})\prod_{j=0}^{N}d\mathbf{r}_j\,d\mathbf{p}_j. \tag{4.3}$$

Taking finer and finer subdivisions of the interval $[t', t]$ and passing to the limit as $N\to\infty$, provided the maximum subinterval for the Nth subdivision $\max\Delta t^{(N)}\to 0$ as $N\to\infty$, we have $G^{(N)}\to G$.

The limit $G^{(N)}$ as $N\to\infty$ with $\max\Delta t^{(N)}\to 0$ is a conditional functional integral in the space of all functions $(\mathbf{r}(\tau), \mathbf{p}(\tau))$ defined over $[t', t]$. We find it natural to adopt the following notation for this functional integral:

$$G(\mathbf{r}|\mathbf{r}',\mathbf{p}|\mathbf{p}';t|t')=\left[\prod_{t'\leqslant\tau<t}\det\{\pi g^{-1}(\tau)\,d\tau\}\right]^{-1/2}$$
$$\times\int\exp\left(-\int_{t'}^{t}g_{\alpha\beta}(\tau)\left[\frac{dp_\alpha(\tau)}{d\tau}-F_\alpha\{\mathbf{r}(\tau),\mathbf{p}(\tau),\tau\}+\{B(\tau)\mathbf{p}(\tau)\}_\alpha\right]\right.$$
$$\left.\times\left[\frac{dp_\beta(\tau)}{d\tau}-\mathbf{F}_\beta\{\mathbf{r}(\tau),\mathbf{p}(\tau),\tau\}+\{B(\tau)\mathbf{p}(\tau)\}_\beta\right]d\tau\right)$$
$$\times\left[\prod_{t'\leqslant\tau<t}\delta\left\{\frac{d\mathbf{r}(\tau)}{d\tau}-m^{-1}\mathbf{p}(\tau)\right\}(d\tau)^3\right]\delta\{\mathbf{r}(t')-\mathbf{r}'\}\delta\{\mathbf{p}(t')-\mathbf{p}'\}$$
$$\times\delta\{\mathbf{r}(t)-\mathbf{r}\}\delta\{\mathbf{p}(t)-\mathbf{p}\}\prod_{t'\leqslant\tau\leqslant t}d\mathbf{r}(\tau)\,d\mathbf{p}(\tau). \tag{4.4}$$

We wish now to express $G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}';\ t|t')$ as a conditional functional integral over momentum functions. To do this we integrate in (4.3) over all $\mathbf{r}_j$ ($j = 0, 1, 2, \ldots, N$) and obtain

$$G^{(N)}=\left[\prod_{j=0}^{N-1}\det\{\pi g^{-1}(t_j)\Delta t_j\}\right]^{-1/2}$$
$$\times\int\exp\left[-\sum_{j=0}^{N-1}g_{\alpha\beta}(t_j)\left\{\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j}-\mathbf{F}\left(\mathbf{r}'+m^{-1}\sum_{k=0}^{j-1}\mathbf{p}_k\Delta t_k,\mathbf{p}_j,t_j\right)+B(t_j)\mathbf{p}_j\right\}_\alpha\right.$$
$$\left.\times\left\{\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{\Delta t_j}-\mathbf{F}\left(\mathbf{r}'+m^{-1}\sum_{k=0}^{j-1}\mathbf{p}_k\Delta t_k,\mathbf{p}_j,t_j\right)+B(t_j)\mathbf{p}_j\right\}_\beta\Delta t_j\right]$$
$$\times\delta\left(\mathbf{r}-\mathbf{r}'-\sum_{j=0}^{N-1}m^{-1}\mathbf{p}_j\Delta t_j\right)\delta(\mathbf{p}_0-\mathbf{p}')\delta(\mathbf{p}_N-\mathbf{p})\prod_{j=0}^{N}d\mathbf{p}_j. \tag{4.5}$$

Again in the limit as $N\to\infty$ with the usual proviso ($\max\Delta t^{(N)}\to 0$) we obtain a conditional functional integral over all momentum functions $\mathbf{p}(\tau)|[t', t]$ with $\mathbf{p}(t') = \mathbf{p}'$ and $\mathbf{p}(t) = \mathbf{p}$. This is another formal expression for the Green function of the Fokker–Planck equation. The notation we adopt here is

$$G(\mathbf{r}|\mathbf{r}',\mathbf{p}|\mathbf{p}',t|t')=\left[\prod_{t'\leqslant\tau<t}\det\{\pi g^{-1}(\tau)\,d\tau\}\right]^{-1/2}$$
$$\times\int\exp\left(-\int_{t'}^{t}g_{\alpha\beta}(\tau)\left[\frac{d\mathbf{p}(\tau)}{d\tau}-\mathbf{F}\left\{\mathbf{r}'+m^{-1}\int_{t'}^{\tau}\mathbf{p}(\tau')\,d\tau',\mathbf{p}(\tau),\tau\right\}\right.\right.$$
$$\left.\left.+B(\tau)\mathbf{p}(\tau)\right]_\alpha\left[\frac{d\mathbf{p}(\tau)}{d\tau}-\mathbf{F}\left\{\mathbf{r}'+m^{-1}\int_{t'}^{t}\mathbf{p}(\tau)\,d\tau,\mathbf{p}(\tau),\tau\right\}+B(\tau)\mathbf{p}(\tau)\right]_\beta d\tau\right)$$
$$\times\delta\left\{\mathbf{r}-\mathbf{r}'-\int_{t'}^{t}m^{-1}\mathbf{p}(\tau)\,d\tau\right\}\delta\{\mathbf{p}(t')-\mathbf{p}'\}\delta\{\mathbf{p}(t)-\mathbf{p}\}\prod_{t'\leqslant\tau\leqslant t}d\mathbf{p}(\tau). \tag{4.6}$$

Finally we wish to find a conditional functional integral over all configuration functions $\mathbf{r}(\tau)|[t', t]$ with $\mathbf{r}(t') = \mathbf{r}'$ and $\mathbf{r}(t) = \mathbf{r}$ to represent the phase-space ECPD. We integrate now over all $\mathbf{p}_j$ ($j = 0, 1, 2, \ldots, N$) in (4.3) and obtain

$$G^{(N)} = \left[\prod_{j=0}^{N-1} \det\{\pi^{-1}m^{-2}g(t_j)\Delta t_j\}\right]^{1/2}$$

$$\times \int \exp\left[-\sum_{j=0}^{N-1} g_{\alpha\beta}(t_j)\left\{m\left(\frac{\mathbf{r}_{j+2}-\mathbf{r}_{j+1}}{\Delta t_{j+1}} - \frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}\right)\Delta t_j^{-1}\right.\right.$$

$$\left. -\mathbf{F}\left(\mathbf{r}_j, m\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}, t_j\right) + B(t_j)m\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}\right\}_\alpha$$

$$\times\left\{m\left(\frac{\mathbf{r}_{j+2}-\mathbf{r}_{j+1}}{\Delta t_{j+1}} - \frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}\right)\Delta t_j^{-1} - \mathbf{F}\left(\mathbf{r}_j, m\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}, t_j\right)\right.$$

$$\left.\left. + B(t_j)m\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{\Delta t_j}\right\}_\beta \Delta t_j\right] \delta(\mathbf{r}_0-\mathbf{r}')\delta\left(\mathbf{p}'-m\frac{\mathbf{r}_1-\mathbf{r}_0}{\Delta t_0}\right)\delta(\mathbf{r}_N-\mathbf{r})$$

$$\times\delta\left(\mathbf{p}-m\frac{\mathbf{r}_{N+1}-\mathbf{r}_N}{\Delta t_N}\right)\left(\frac{m}{\Delta t_N}\right)^3 \prod_{j=0}^{N+1} d\mathbf{r}_j. \tag{4.7}$$

The change in the normalization factor of (4.7) is due to the integrations over the $\mathbf{p}_j$, which appear in the δ functions of (4.3). The introduction of the new variable of integration $\mathbf{r}_{N+1}$ is to ensure the condition $\mathbf{p}(t) = \mathbf{p}$. Again passing to the limit as $N \to \infty$ with $\max \Delta t^{(N)} \to 0$, we have a conditional functional integral over all configuration functions $\mathbf{r}(\tau)|[t', t]$ with $\mathbf{r}(t') = \mathbf{r}'$, $\mathbf{r}(t) = \mathbf{r}$ representing the ECPD in phase space. The notation we use to represent G through the above limiting process is

$$G(\mathbf{r}|\mathbf{r}', \mathbf{p}|\mathbf{p}'; t|t') = \left[\prod_{t'\leqslant\tau<t} \det\{\pi^{-1}m^{-2}g(\tau)\,d\tau\}\right]^{1/2}$$

$$\times \int \exp\left(-\int_{t'}^{t} g_{\alpha\beta}(\tau)[m\ddot{\mathbf{r}}(\tau) - \mathbf{F}\{\mathbf{r}(\tau), m\dot{\mathbf{r}}(\tau), \tau\} + B(\tau)m\dot{\mathbf{r}}(\tau)]_\alpha\right.$$

$$\left.\times[m\ddot{\mathbf{r}}(\tau) - \mathbf{F}\{\mathbf{r}(\tau), m\dot{\mathbf{r}}(\tau), \tau\} + B(\tau)m\dot{\mathbf{r}}(\tau)]_\beta\, d\tau\right)$$

$$\times\delta\{\mathbf{r}(t')-\mathbf{r}'\}\delta\{\mathbf{p}'-m\dot{\mathbf{r}}(t')\}\delta\{\mathbf{r}(t)-\mathbf{r}\}\delta\{\mathbf{p}-m\dot{\mathbf{r}}(t)\}\left(\frac{m}{dt}\right)^3 \prod_{t'\leqslant\tau\leqslant t+0} d\mathbf{r}(\tau). \tag{4.8}$$

The dots upon $\mathbf{r}$ in (4.8) denote as usual differentiation with respect to τ. $t+0$ under the product symbol stands for the extra variable of integration in the limiting process.

It is worth noting that the quantity in the square brackets of the exponential function in (4.8) is the left-hand side of the Langevin equation in terms of $\mathbf{r}$ if on the right-hand side we have only the thermal force. Similar remarks apply to the exponential expressions in the functional integrals (4.4) and (4.6).

It is interesting to note that one could obtain the result (4.8) from the functional integral (2.4) over all collision force functions by change of the variable of integration through the Langevin equation (1.1) after eliminating $\mathbf{p}(\tau)$ through (1.2). But there is a point to which attention should be drawn in transformations involving continuous functionals, that of the Jacobian of the transformation. The Jacobian is obtained by going over to the discrete case and then passing to the limit of continuality. It so happens that the various ways of approximating continuous functionals by discrete ones yield in general different Jacobians.†

† I am grateful to Professor S. F. Edwards for drawing my attention to this peculiarity.

Mathematically one obtains unique results for the Green function, as far as the normalization factor is consistent with the approximating expressions employed. In our definitions of the functional integrals (4.4), (4.6) and (4.8) we have chosen the approximating expressions indicated in (4.3), (4.5) and (4.7) for two reasons: mathematical simplicity, and for a physical reason which is related to causality as follows.

For instance, in the approximate expression (4.3) for the Green function G the right-hand side is built up from Green functions connecting the neighbouring times t_j, t_{j+1} ($t_{j+1} > t_j$). These Green functions when chosen as in (4.2) multiplied by $\delta(\mathbf{r}_{j+1}-\mathbf{r}_j-m^{-1}\mathbf{p}_j\Delta t_j)$ have the interpretation of being the transition probability densities for the particle at the phase point $(\mathbf{r}_j, \mathbf{p}_j)$ at time t_j to find itself at a later time t_{j+1} in the vicinity of the phase point $(\mathbf{r}_{j+1}, \mathbf{p}_{j+1})$ under the action of force depending on the values $\mathbf{r}_j$, $\mathbf{p}_j$ of the particle position and momentum at time t_j. This situation looks perfectly natural. If we employ an alternative approximation to (1.1a, b), for example

$$\frac{\mathbf{p}_{j+1}-\mathbf{p}_j}{t_{j+1}-t_j}+B(t_{j+1})\mathbf{p}_{j+1}-\mathbf{F}(\mathbf{r}_{j+1}, \mathbf{p}_{j+1}, t_{j+1}) = \mathbf{f}(t_{j+1}) \tag{4.9}$$

$$\mathbf{p}_{j+1} = m\frac{\mathbf{r}_{j+1}-\mathbf{r}_j}{t_{j+1}-t_j} \tag{4.10}$$

the interpretation of the resulting Green function connecting the neighbouring times t_j, t_{j+1} would be the transition probability density for the particle being at the phase point $(\mathbf{r}_j, \mathbf{p}_j)$ at time t_j to change to $(\mathbf{r}_{j+1}, \mathbf{p}_{j+1})$ at time t_{j+1} under the action of forces depending on the 'probable' phase point $(\mathbf{r}_{j+1}, \mathbf{p}_{j+1})$ to be occupied by the particle at the later time t_{j+1}.

The expressions (4.6) and (4.8) were also derived by Onsager and Machlup (1953) without the crucial normalization factor, and in the particular case of the free Brownian particle. Next we shall show how to extract explicit expressions for the Green function from the functional representations.

5. Approximation methods for the Green function

The various functional integral representations of the Green function of the Fokker–Planck equation are not only formal devices, but their practical importance lies in the fact that they can be used in approximation procedures. The technique consists of employing a transformation of $\mathbf{r}(\tau)$, $\mathbf{p}(\tau)$, which transforms part of the integral into a functionally known integrable form. The rest can be treated as a perturbation.

One particular scheme, which in certain circumstances picks up most of the Green function in the zeroth-order approximation, is analogous to the WKB approximation in quantum mechanics (see e.g. Feynman and Hibbs 1965). In I we demonstrated this technique by treating the one-dimensional momentum Green function in the case where the force is independent of the particle position. In the present work we wish to generalize the method to the three-dimensional case. Again we shall consider the external force to be of the form $\mathbf{F}(\mathbf{p}, \tau)$. In this case it is meaningful to ask for the ECPD in momentum space, $G(\mathbf{p}|\mathbf{p}'; t|t')$. Its functional integral representation over momentum functions obtained from the ECPD in phase space (4.4) by integrating over all $\mathbf{r}(\tau)|[t', t]$ is

$$\begin{aligned} G(\mathbf{p}|\mathbf{p}'; t|t') = {} & \left[\det\left\{\prod_{t'\leqslant\tau<t} \pi g^{-1}(\tau)\, d\tau\right\}\right]^{-1/2} \\ & \times \int \exp\left(-\int_{t'}^{t} g_{\alpha\beta}(\tau)\left[\frac{d\mathbf{p}(\tau)}{d\tau}-\mathbf{F}\{\mathbf{p}(\tau), \tau\}+B(\tau)\mathbf{p}(\tau)\right]_\alpha\right. \\ & \left.\times\left[\frac{d\mathbf{p}(\tau)}{d\tau}-\mathbf{F}\{\mathbf{p}(\tau), \tau\}+B(\tau)\mathbf{p}(\tau)\right]_\beta d\tau\right) \\ & \times\delta\{\mathbf{p}(t')-\mathbf{p}'\}\delta\{\mathbf{p}(t)-\mathbf{p}\}\prod_{t'\leqslant\tau\leqslant t} d\mathbf{p}(\tau). \end{aligned} \tag{5.1}$$

From the positive definiteness of g it follows that the exponential argument in (5.1) is positive for every path $\mathbf{p}(\tau)$. For 'smooth' $\mathbf{F}(\mathbf{p}, \tau)$ with respect to $\mathbf{p}$ there exists a certain path through $(t', \mathbf{p}')$ and $(t, \mathbf{p})$ for which the exponential argument is minimized and therefore the exponential functional is maximized. Then most of the contribution to the functional integral (5.1) from the integrations over $\mathbf{p}(\tau)|[t', t]$ comes from a neighbourhood around the minimizing path. To find this path we apply the usual methods of the calculus of variations. We shall consider the case of constant g as this is the usual case for applications.

We have, for the required path using matrix notation,

$$\delta \int_{t'}^{t} \{\dot{\tilde{\mathbf{p}}} + \tilde{\mathbf{p}}\tilde{B} - \tilde{\mathbf{F}}(\mathbf{p}, \tau)\} g \{\dot{\mathbf{p}} + B\mathbf{p} - \mathbf{F}(\mathbf{p}, \tau)\}\, d\tau = 0 \tag{5.2}$$

together with the conditions

$$\mathbf{p}(t') = \mathbf{p}', \qquad \mathbf{p}(t) = \mathbf{p}. \tag{5.2a}$$

Owing to the symmetry of the matrix g one can perform the variation either with respect to $\mathbf{p}$ or its transpose $\tilde{\mathbf{p}}$. Thus, for the minimizing trajectory, the Euler–Lagrange equation is of the second order in the time ordinary vector differential equation:

$$\ddot{\mathbf{p}} + \left\{B\left(\widetilde{\frac{\partial \mathbf{F}}{\partial \mathbf{p}}}\right)B^{-1} - \frac{\partial \mathbf{F}}{\partial \mathbf{p}}\right\}\dot{\mathbf{p}} - \frac{\partial \mathbf{F}}{\partial \tau} - B^2\mathbf{p} + B\mathbf{F} + B\left(\widetilde{\frac{\partial \mathbf{F}}{\partial \mathbf{p}}}\right)(\mathbf{p} - B^{-1}\mathbf{F}) = 0. \tag{5.3}$$

For the derivation of this equation we have taken into account the relation $g^{-1} = 4\kappa TmB$ and the symmetry of B. Equation (5.3) is in general non-linear. However, being an ordinary differential equation it is easier to tackle than a partial one. Let $\mathbf{p}^*(\tau)$ be the solution of (5.3) which satisfies (5.2a). Introducing the transformation

$$\mathbf{p}(\tau) = \mathbf{p}^*(\tau) + \mathbf{q}(\tau) \tag{5.4}$$

we have

$$\begin{aligned}\int_{t'}^{t} &\{\dot{\tilde{\mathbf{p}}} + \tilde{\mathbf{p}}\tilde{B} - \tilde{\mathbf{F}}(\mathbf{p}, \tau)\} g \{\dot{\mathbf{p}} + B\mathbf{p} - \mathbf{F}(\mathbf{p}, \tau)\}\, d\tau \\ &= \int_{t'}^{t} \tilde{\mathbf{A}}(\tau) g \mathbf{A}(\tau)\, d\tau + \int_{t'}^{t} \{\dot{\tilde{\mathbf{q}}}(\tau) g \dot{\mathbf{q}}(\tau) + \tilde{\mathbf{q}}(\tau)\alpha(\tau) g \dot{\mathbf{q}}(\tau) + \dot{\tilde{\mathbf{q}}}(\tau) g \tilde{\alpha}(\tau)\mathbf{q}(\tau)\}\, d\tau \\ &\quad + \int_{t'}^{t} \tilde{\mathbf{q}}(\tau) C(\tau) \mathbf{q}(\tau)\, d\tau + \mathrm{O}\{\mathbf{q}^3(\tau)\}.\end{aligned} \tag{5.5}$$

The first-order term in $\mathbf{q}(\tau)$ in (5.5) vanishes, since this is the first variation of the left-hand side, which has been taken as zero in (5.2). If the external force $\mathbf{F}$ is at most linearly dependent on $\mathbf{p}$, then the calculation of the Green function with this procedure is exact. We have adopted the following notation:

$$\mathbf{A}(\tau) = \dot{\mathbf{p}}^* - \mathbf{F}(\mathbf{p}^*, \tau) + B\mathbf{p}^* = \mathbf{A}(\mathbf{p}, \mathbf{p}'; \tau) \tag{5.6a}$$

$$\alpha(\tau) = B - \left(\frac{\partial \mathbf{F}}{\partial \mathbf{p}}\right)^* = \alpha(\mathbf{p}, \mathbf{p}'; \tau) \tag{5.6b}$$

$$C(\tau) = \tilde{\alpha}(\tau) g \alpha(\tau) - \tfrac{1}{2}\left\{\tilde{\mathbf{A}}(\tau) g \left(\frac{\partial^2 \mathbf{F}}{\partial \mathbf{p}\,\partial \mathbf{p}}\right)^*\right\} - \tfrac{1}{2}\left\{\left(\widetilde{\frac{\partial^2 \mathbf{F}}{\partial \mathbf{p}\,\partial \mathbf{p}}}\right)^* g \mathbf{A}(\tau)\right\} = C(\mathbf{p}, \mathbf{p}', \tau). \tag{5.6c}$$

The asterisk on quantities in parentheses means that they are evaluated at $\mathbf{p}(\tau) = \mathbf{p}^*(\tau)$. The notation

$$\left\{\tilde{\mathbf{A}} g \left(\frac{\partial^2 \mathbf{F}}{\partial \mathbf{p}\,\partial \mathbf{p}}\right)^*\right\}_{\lambda\mu}$$

stands for

$$A_\alpha g_{\alpha\beta}\left(\frac{\partial^2 \mathbf{F}_\beta}{\partial p_\lambda \partial p_\mu}\right)^*.$$

It is easy to establish that the matrix $C(\tau)$ defined in (5.6*c*) is symmetric. The Jacobian of the functional transformation $\mathbf{p} \to \mathbf{q}$ is $J(\mathbf{p} \to \mathbf{q}) = 1$. Furthermore, owing to (5.2*a*) it follows

$$\mathbf{q}(t') = \mathbf{q}(t) = 0. \tag{5.7}$$

Therefore we have for the Green function the result

$$\begin{aligned} G(\mathbf{p}|\mathbf{p}'; t|t') &\simeq G_0(\mathbf{p}|\mathbf{p}'; t|t') \\ &= \exp\left\{-\int_{t'}^{t} \tilde{\mathbf{A}}(\tau) g \mathbf{A}(\tau)\, d\tau\right\} \times \left\{\prod_{t' \leqslant \tau < t} \det(\pi g^{-1}\, d\tau)\right\}^{-1/2} \\ &\quad \times \int \exp\left\{-\int_{t'}^{t} [\dot{\tilde{\mathbf{q}}}(\tau) g \dot{\mathbf{q}}(\tau) + \tilde{\mathbf{q}}(\tau)\tilde{\alpha}(\tau) g \dot{\mathbf{q}}(\tau) + \dot{\tilde{\mathbf{q}}}(\tau) g \alpha(\tau)\mathbf{q}(\tau) + \tilde{\mathbf{q}}(\tau) C(\tau)\mathbf{q}(\tau)]\, d\tau\right\} \\ &\quad \times \delta\{\mathbf{q}(t') - \mathbf{0}\}\delta\{\mathbf{q}(t) - \mathbf{0}\} \prod_{t' \leqslant \tau \leqslant t} d\mathbf{q}(\tau). \end{aligned} \tag{5.8}$$

The approximation sign in (5.8) is due to the omission of the higher powers in $\mathbf{q}$.

To calculate the continual Gaussian integral (5.8) we pass to the discrete form. Let us then consider a partition of the interval $[t', t]$:

$$\mathscr{D}_N = \{t_0, t_1, t_2, \ldots, t_N\}$$

with

$$t' = t_0 < t_1 < t_2 < \ldots < t_N = t.$$

For simplicity we shall take the partition $\mathscr{D}_N$ isomeric, i.e. $t_{j+1} - t_j = \Delta\tau$ for $j = 0, 1, 2, \ldots, N-1$. Then we form the expression $G_0^{(N)}$ by replacing the integrals and symbolic products in (5.8) by the corresponding sums and products over the points of the partition $\mathscr{D}_N$. Denoting by S the argument of the exponential function in the functional integral (5.8), we have for the discrete form of the functional S the sum

$$\begin{aligned} S_N &= \frac{1}{\Delta\tau}\sum_{j=0}^{N-1} \{(\tilde{\mathbf{q}}_{j+1} - \tilde{\mathbf{q}}_j) g (\mathbf{q}_{j+1} - \mathbf{q}_j) + \Delta\tau \tilde{\mathbf{q}}_j \tilde{\alpha}_j g (\mathbf{q}_{j+1} - \mathbf{q}_j) \\ &\qquad + \Delta\tau (\tilde{\mathbf{q}}_{j+1} - \tilde{\mathbf{q}}_j) g \alpha_j \mathbf{q}_j + (\Delta\tau)^2 \tilde{\mathbf{q}}_j C_j \mathbf{q}_j\} \\ &= \frac{1}{\Delta\tau}\sum_{j=0}^{N-1} \{\tilde{\mathbf{q}}_j [2g - \Delta\tau(\tilde{\alpha}_j g - g\alpha_j) + (\Delta\tau)^2 C_j]\mathbf{q}_j \\ &\qquad - \tilde{\mathbf{q}}_j (g - \Delta\tau \tilde{\alpha}_j g)\mathbf{q}_{j+1} - \tilde{\mathbf{q}}_{j+1}(g - \Delta\tau\alpha_j)\mathbf{q}_j\} \end{aligned} \tag{5.9}$$

where in (5.9) we have taken into account the condition (5.7), which in the discrete case reads

$$\mathbf{q}_0 = \mathbf{q}_N = \mathbf{0}.$$

Here again we have denoted $\alpha(t_j)$, $C(t_j)$ and $\mathbf{q}(t_j)$ by α_j, C_j and $\mathbf{q}_j$. S_N is easily seen to be symmetric with respect to $\mathbf{q}_j$, $\mathbf{q}_{j+1}$. On account of this symmetry it is possible to transform (5.9) by a principal axis transformation, originally employed by Abé (1954) for Gaussian functional integrals. We try to cast (5.9) in the form

$$S_N = \frac{1}{\Delta\tau}\sum_{j=1}^{N-1} (\tilde{\mathbf{q}}_j - \tilde{\mathbf{q}}_{j+1}\tilde{b}_{j+1})\Lambda_j(\mathbf{q}_j - b_{j+1}\mathbf{q}_{j+1}) \tag{5.10}$$

with $\mathbf{q}_N = \mathbf{0}$.

$$b_2, b_3, \ldots, b_{N-1}; \qquad \Lambda_1, \Lambda_2, \ldots, \Lambda_{N-1}$$

are 3×3 matrices. The Λ matrices are taken symmetric. It is possible now to rearrange (5.10) in the form of (5.9) and there by comparison to obtain

$$\Lambda_1 = 2g-\Delta\tau(\tilde{\alpha}_1 g+g\alpha_1)+(\Delta\tau)^2C_1 \tag{5.11a}$$

$$\Lambda_{j+1}+\tilde{b}_{j+1}\Lambda_j b_{j+1} = 2g-\Delta\tau(\alpha_{j+1}g+g\alpha_{j+1})+(\Delta\tau)^2C_{j+1} \quad (j=1,2,\ldots,N-2) \tag{5.11b}$$

$$\Lambda_j b_{j+1} = (I-\Delta\tau\alpha_j)g, \qquad \tilde{b}_{j+1}\Lambda_j = g(I-\Delta\tau\alpha_j) \quad (j=1,2,\ldots,N-1) \tag{5.11c}$$

The symmetry of Λ_j renders the equations (5.11c) consistent. From (5.11) we obtain

$$b_{j+1} = \Lambda_j^{-1}(I-\Delta\tau\alpha_j)g$$

$$\Lambda_{j+1}+g(I-\Delta\tau\alpha_j)\Lambda_j^{-1}(I-\Delta\tau\tilde{\alpha}_j)g-2g+\Delta\tau(\tilde{\alpha}_{j+1}g+g\alpha_{j+1})-(\Delta\tau)^2C_{j+1} = 0$$

$$(j=1,2,\ldots,N-2). \tag{5.12}$$

We make a further substitution:

$$\boldsymbol{\xi}_j = \mathbf{q}_j-b_{j+1}\mathbf{q}_{j+1} \quad \text{for} \quad (j=1,2,\ldots,N-2)$$
$$\boldsymbol{\xi}_{N-1} = \mathbf{q}_{N-1}. \tag{5.13}$$

Again the Jacobian of the transformation $\mathbf{q}\to\boldsymbol{\xi}$ is

$$J(\mathbf{q}\to\boldsymbol{\xi}) = 1.$$

Employing (5.13), we write (5.10) as

$$S_N = \frac{1}{\Delta\tau}\sum_{j=1}^{N-1}\tilde{\boldsymbol{\xi}}_j\Lambda_j\boldsymbol{\xi}_j. \tag{5.14}$$

With the aid of (5.14) the discrete form of (5.8) becomes

$$G_0^{(N)} = \exp\left\{-\int_{t'}^{t}\tilde{\mathbf{A}}(\tau)g\mathbf{A}(\tau)\,d\tau\right\}.\left\{\prod_{j=0}^{N-1}\det(\pi g^{-1}\Delta\tau)\right\}^{-1/2}$$
$$\times\int\exp\left(-\frac{1}{\Delta\tau}\sum_{j=1}^{N-1}\tilde{\boldsymbol{\xi}}_j\Lambda_j\boldsymbol{\xi}_j\right)\prod_{j=1}^{N-1}d\boldsymbol{\xi}_j. \tag{5.15}$$

Performing the integrations over $\boldsymbol{\xi}_j$ we obtain

$$G_0^{(N)} = \{\det(\pi^{-1}g)\}^{1/2}\left[\det\left\{(\Delta\tau)\prod_{j=1}^{N-1}g^{-1}\Lambda_j\right\}\right]^{1/2}\exp\left\{-\int_{t'}^{t}\tilde{\mathbf{A}}(\tau)g\mathbf{A}(\tau)\,d\tau\right\}. \tag{5.16}$$

Although the matrices $g^{-1}\Lambda_j$ ($j=1,2,\ldots,N-1$) do not commute in general, the value of the determinant of their product is independent of their order. We define

$$D_n = \Delta\tau g^{-1}\Lambda_1 g^{-1}\Lambda_2\ldots g^{-1}\Lambda_{n-1} = \Delta\tau\prod_{j=1}^{n-1}g^{-1}\Lambda_j. \tag{5.17}$$

What we need now for passing to the $\lim G_0^{(N)}$ as $N\to\infty$ is to find

$$\lim_{N\to\infty\ (\text{or } \Delta\tau\to\infty)} D_N = D(t) = D(\mathbf{p},\mathbf{p}';t,t'). \tag{5.18}$$

To this end we shall develop a differential equation for $D(\tau) = \lim D_n$, as $n\to\infty$. Let us consider an $(n+1)$-point partition of the interval $[t',\tau]$, $\Delta\tau$ being $(\tau-t')/n$. By (5.17) we have the relation

$$D_{n+1} = D_n g^{-1}\Lambda_n. \tag{5.19}$$

Let us write the second identity of (5.12), as applied to the interval $[t', \tau]$, as follows:

$$g^{-1}\Lambda_n + (I - \Delta\tau\alpha_{n-1})\Lambda_{n-1}{}^{-1}(I - \Delta\tau\tilde{\alpha}_{n-1})g - 2I + (\Delta\tau)g^{-1}(\tilde{\alpha}_n g + g\alpha_n) - (\Delta\tau)^2 g^{-1}C_n = 0. \tag{5.20}$$

Multiplying (5.20) on the left by D_n and taking into account (5.19) we can write

$$\begin{aligned}&\frac{D_{n+1} - 2D_n + D_{n-1}}{(\Delta\tau)^2} + \frac{D_n g^{-1}\tilde{\alpha}_n g - D_{n-1}g^{-1}\tilde{\alpha}_{n-1}g}{\Delta\tau} \\ &+ D_n \frac{\alpha_n D_{n-1}{}^{-1} - \alpha_{n-1}D_{n-1}{}^{-1} + \alpha_{n-1}D_{n-1}{}^{-1} - \alpha_{n-1}D_n{}^{-1}}{\Delta\tau} D_{n-1} \\ &+ D_n(\alpha_{n-1}D_n{}^{-1}D_{n-1}g^{-1}\tilde{\alpha}_{n-1}g - g^{-1}C_n) = 0.\end{aligned} \tag{5.21}$$

Passing to the limit as $\Delta\tau \to 0$ (or, what is the same, $n \to \infty$) we obtain the following matrix ordinary differential equation for $D(\tau)$:

$$\frac{d^2D}{d\tau^2} + \frac{d}{d\tau}(Dg^{-1}\tilde{\alpha}g) + D\frac{d\alpha}{d\tau} + D\alpha D^{-1}\frac{dD}{d\tau} + D(\alpha g^{-1}\tilde{\alpha}g - g^{-1}C) = 0 \tag{5.22}$$

where for the derivation of (5.22) we have utilized the identity

$$-\frac{dD^{-1}}{d\tau}D = D^{-1}\frac{dD}{d\tau}.$$

In the one-dimensional case equation (5.22) is linear because there α and D commute. Therefore the non-linear term

$$D\alpha D^{-1}\dot{D} \quad \text{becomes} \quad \alpha\dot{D}.$$

The required $D(t)$ is the solution of (5.22) evaluated at $\tau = t$, and which satisfies the initial conditions

$$D(0) = 0, \qquad \dot{D}(0) = I \tag{5.23}$$

since

$$D_1 = \Delta\tau\{2I - \Delta\tau(g^{-1}\tilde{\alpha}_1 g + \alpha_1) + (\Delta\tau)^2 C_1\} \to 0, \quad \text{as} \quad \Delta\tau \to 0$$

and

$$\frac{D_2 - D_1}{\Delta\tau} \to I, \quad \text{as} \quad \Delta\tau \to 0.$$

Actually we are interested in the determinant of $D(t)$. One may notice that, by choosing a different ordering of the matrices $g^{-1}\Lambda_j$ for the definition of D, we would produce an alternative differential equation for D. However, the determinant of the new D remains invariant under the same initial conditions.

From (5.16) and (5.17) we obtain the following approximate result in compact form for the Green function:

$$\begin{aligned}\lim_{N\to\infty} G_0{}^{(N)} &= G_0(\mathbf{p}|\mathbf{p}'; t|t') \\ &= [\det\{\pi g^{-1}D(\mathbf{p}, \mathbf{p}'; t, t')\}]^{-1/2} \exp\left\{-\int_{t'}^{t} \tilde{\mathbf{A}}(\mathbf{p}, \mathbf{p}', \tau)g\mathbf{A}(\mathbf{p}, \mathbf{p}', \tau)\, d\tau\right\}.\end{aligned} \tag{5.24}$$

This result can be taken as a zero-order approximation to G. We can further improve the approximation by expanding the rest of the exponential functional in (5.1) in power series of $\mathbf{q}$ and subsequently by transformation in $\boldsymbol{\xi}$ and employ the measure in (5.15) for the averaging over the $\boldsymbol{\xi}$'s.

Onsager and Machlup considered the one-dimensional case of a free Brownian particle and produced the analogue of the exponential expression in (5.24) (which is exact when $\mathbf{F}=0$ or at most linearly dependent on $\mathbf{p}$) but they did not calculate the factor in front of the exponential function. This factor in the general case is not a normalization factor, but it is part of the probability function since it depends on $\mathbf{p}$ as well.

6. Conclusion

The functional approach to the problem of Brownian motion seems extremely appropriate for theoretical investigations. It is also useful for solving the Fokker–Planck equation in the case of non-linear Brownian motion. However, this approach in its present stage is limited to the case of infinite media.

Acknowledgments

The author would like to thank Professor S. F. Edwards for very helpful discussions which enabled him to clarify certain points in the present work.

References

Abé, R., 1954, *Busseiron Kenk-yu*, **79**, 101.
Chandrasekhar, S., 1943, *Rev. Mod. Phys.*, **15**, 1.
Edwards, S. F., 1964, *J. Fluid Mech.*, **18**, 239.
Einstein, A., 1956, *Investigations on the Theory of Brownian Movement* (New York: Dover Publications), p. 1.
Feynman, R. P., and Hibbs, A. R., 1965, *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill), pp. 58–61.
Landau, L. D., and Lifshitz, E. M., 1959, *Fluid Mechanics* (Oxford: Pergamon Press), pp. 67, 97.
Onsager, L., and Machlup, S., 1953, *Phys. Rev.*, **91**, 1505.
Papadopoulos, G. J., 1967, *Lectures in Theoretical Physics* (Boulder: University of Colorado Press).
Perrin, J., 1916, *Atoms* (London: Constable).