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Eigentheory of the Inhomogeneous Fokker–Planck Equation

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Ambiguities that occur in the existing eigentheory of the inhomogeneous Fokker–Planck equation are resolved. The eigenfunction expansion is shown to be identical to the known exact solution, generalizing an earlier result for the space-homogeneous case.

KEY WORDS: Fokker–Planck equation; eigentheory; Brownian motion.

There are a number of nonequilibrium problems that can be studied by using a perturbative approach using infinite-dilution Brownian motion for the reference propagator.[3] The mathematical theory for describing the infinite-dilution Brownian motion is well developed,[(5)] and has proven capable of accommodating certain recent generalizations.[(6)] In the present paper we will be concerned with solutions to the inhomogeneous Fokker–Planck equation (IFPE), which we define here to avoid ambiguity to be the kinetic equation that describes the distribution function $f(\mathbf{r}, \mathbf{p}, t)$ for a Brownian particle at infinite dilution. For the spatially uniform case the fundamental solution of this equation was found by Uhlenbeck and Ornstein.[(7)] The eigentheory for this case is implicit in their results,[4] and an explicit eigentheory has also been given.[(8)] The fundamental solution for the IFPE is also known [Ref. 5,

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[3] The pioneering work of Friedman together with recent extensions remains the most ambitious attempt at doing this.[(1)] For a recent extension see Degani.[(2)] Also, in a different context, Mazo[(3)] and Harris.[(4)]

[4] See note II at the end of Ref. 7.

Sections 4(ii), 4(iii)], and more recently an eigentheory for this equation has been considered.[9] In our own work in progress, on separate problems, we have attempted to use this eigentheory and have concluded that the existing treatment is somewhat ambiguous. The purpose of this note is to give a clear exposition of the theory, which we hope others will find useful.

The notation used here will follow that of Refs. 1 and 9 with only minor changes. The IFPE is

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m}\cdot\frac{\partial f}{\partial \mathbf{r}} = \zeta \frac{\partial}{\partial \mathbf{p}}\cdot\left(\beta^{-1}\frac{\partial}{\partial \mathbf{p}} + \frac{\mathbf{p}}{m}\right)f \tag{1}$$

with $\beta = 1/k_BT$ and ζ the friction coefficient. The fundamental solution to this equation has been given by Chandrasekhar [Ref. 5, Sections 4(ii), 4(iii)], using methods from the theory of differential equations. For convenience we will work directly with the Fourier transform of f,

$$f_{\mathbf{q}}(\mathbf{p}, t) \equiv \int d\mathbf{r}\, \exp(i\mathbf{q}\cdot\mathbf{r})\, f(\mathbf{r}, \mathbf{p}, t) \tag{2}$$

in which case we can take the initial coordinate to be the origin. From Ref. 1 we have

$$f_{\mathbf{q}}(\mathbf{p}, t) = (\pi G)^{-3/2} \exp[-S^2/G - q^2D/4G + i\mathbf{q}H\cdot(\mathbf{p} + \mathbf{p}_0)/G] \tag{3}$$

where $\mathbf{p}_0$ is the initial value of $\mathbf{p}$, and

$$\begin{aligned} &\mathbf{S} = \mathbf{p} - \mathbf{p}_0\theta, \qquad \theta = e^{-t\zeta/m} \\ &G = 2m\beta^{-1}[1 - \theta^2], \qquad H = (2m/\beta\zeta)[1 - \theta]^2 \\ &D = FG - H^2, \qquad F = (2m/\beta\zeta^2)[2(t/m)\zeta - 3 + 4\theta - \theta^2] \end{aligned} \tag{4}$$

Since the solution separates, we will restrict ourselves to the one-dimensional problem in what follows.

In going from Eq. (3) to the final result of this section only a transformation of variables and algebraic manipulation is required. Some insight as to how to proceed is provided by earlier work[9]; however, our conclusions will be seen to be somewhat different than those results. In terms of the reduced variables k and u, where

$$k(2\beta/m)^{1/2}\zeta = q, \qquad u(2m/\beta)^{1/2} = p \tag{5}$$

we have

$$f_k(u, t) = (\pi\bar{G})^{-1/2} \exp\{\bar{G}^{-1}[-u^2 - \theta^2u_0^2 + 2\theta uu_0 - k^2\bar{D} + 2ik(u + u_0)\bar{H}]\} \tag{6}$$

where $\bar{G}$, $\bar{H}$, and $\bar{F}$ are defined as the appropriate bracketed terms in Eq. (4)

(e.g., $\bar{G} = 1 - \theta^2$) and $\bar{D} = \bar{F}\bar{G} - \bar{H}^2$. In terms of these variables and $z = u - 2ik$, $z_0 = u_0 - 2ik$ the above expression can be written as

$$f_k(u, t) = (\pi\bar{G})^{-1/2} \exp(u_0^2 + 2k^2) \exp(-2t\zeta k^2/m) \exp[-(u - ik)^2] \\ \times \exp[-(u_0 - ik)^2] \exp[-\bar{G}^{-1}(z^2 + z_0^2 - 2zz_0\theta)] \exp(z^2 + z_0^2) \tag{7}$$

Making use of an identity for Hermite polynomials,[(10),5] we then arrive at

$$f_k(u, t) = \pi^{-1/2} \exp(u_0^2 + 2k^2) \exp(-2t\zeta k^2/m) \\ \times \exp[-(u - ik)^2] \exp[-(u_0 - ik)^2] \\ \times \sum_{n=0}^{\infty} (\theta^n/2^n n!) H_n(z) H_n(z_0) \tag{8}$$

which suggests the eigenfunction expansion

$$f_k(u, t) = \sum_n c_n(k, t)\psi_n(k, u) \tag{9}$$

with eigenfunctions $\psi_n(k, u) = \{\exp[-(u - ik)^2]\}H_n(u - 2ik)$.

The eigenvalue problem associated with the Fourier-transformed IFPE is

$$\left[piq + \zeta \frac{\partial}{\partial p}\left(\beta^{-1}\frac{\partial}{\partial p} + \frac{p}{m}\right)\right]\psi_n(q, p) = \Lambda_n(q)\psi_n(q, p) \tag{10}$$

This differs in the sign of the term containing the i from the corresponding equation studied in Ref. 9 [cf. Eq. (A4.18) there]. This is a minor point, but taken together with a misprint in the final result there, Eq. (A4.29), it leads to an uncertainty as to the precise specification of the eigenfunctions. The key issue is orthogonality, and as we shall show, the ψ_n are themselves orthogonal, with respect to the proper weight function, rather than conjugate pairs as might be expected.

In terms of the reduced variables u, k and reduced eigenvalues

$$\mu_n(k) = (m/\zeta)\Lambda_n(k) \tag{11}$$

Eq. (10) becomes

$$\left[2uik + \frac{\partial}{\partial u}\left(\frac{1}{2}\frac{\partial}{\partial u} + u\right) - \mu_n\right]\psi_n = 0 \tag{12}$$

Now let

$$\psi_n = \{\exp[-(u - ik)^2]\}\phi_n(u, k) \tag{13}$$

[5] The identity used to go from Eq. (7) to Eq. (8) does not appear in several other standard reference sources for mathematical formulas, so the misprint in the sign of the denominator that appears here is particularly vexatious. The correct form follows from the results of note II of Ref. 7 when Hermite polynomials are used in place of the Weber's functions used there, and also directly from the generating function formula for Hermite polynomials.

and use $z = u - 2ik$ again, so that Eq. (12) can be written as

$$\frac{\partial^2\phi_n}{\partial z^2} - 2z\frac{\partial\phi_n}{\partial z} + 2n\phi_n = 0 \tag{14}$$

where

$$\mu_n = -n - 2k^2 \tag{15}$$

This differs from Ref. 9, in which the coefficient of the k^2 term is 1, but agrees with our earlier result, Eq. (7). The substitution given in Eq. (13) and subsequent transformation from u, k to z, which are both taken directly from Ref. 9, are the crucial elements that allow us essentially to solve Eq. (12) by inspection since in this representation we need only solve Eq. (14), which is the canonical equation for Hermite polynomials $H_n(z)$,[6] so that

$$\psi_n = \{\exp[-(u - ik)^2]\}H_n(u - 2ik) \tag{16}$$

Returning now to the Fourier-transformed IFPE, with our use of reduced variables continued, the standard procedure for solving this equation is to expand $f_k(u, t)$ in the ψ_n, as shown in Eq. (9). If the equation is not Hermitian adjoint, the eigenfunctions for the Hermitian adjoint equation must be used or else the c_n cannot be determined by the usual argument, which depends on the orthogonality of the eigenfunctions. But we know that the H_n are orthogonal on the real axis, and so we would not expect the difficulties with such an expansion indicated in Ref. 9. Let us first show this and then see why this is the case. Substituting Eq. (9) into the Fourier transform of Eq. (1) written in terms of u and k, and multiplying by $\psi_m \exp(u^2 + 2k^2)$ and integrating over z, we obtain

$$\sum_n \left(\frac{\partial c_n}{\partial t} - \Lambda_n c_n\right)\int_{-\infty}^{\infty} dz\, e^{-z^2}H_m(z)H_n(z) = 0 \tag{17}$$

from which it follows that

$$c_n(k, t) = c_n(k, 0)\exp(-n\zeta t/m - 2k^2 t\zeta/m) \tag{18}$$

Using Eq. (9) at $t = 0$, we find in the same way

$$c_n(k, 0) = \{\exp(u_0{}^2 + 2k^2)\exp[-(u_0 - ik)^2]\}H_n(z_0)/\pi^{1/2}2^n n! \tag{19}$$

so that Eqs. (9), (15), (18), and (19) give the identical result as Eq. (8)!

[6] If we use $k' = 2^{1/2}k$, $u' = 2^{1/2}u$ in place of k and u and let

$$\psi_n = \{\exp[-(u' - ik')^2/2]\}\phi_n'(k', u'),$$

then we find $\phi_n' = He_n(z')$ and $\mu_n' = -n - k'^2$. This choice of reduced variables allows the three-dimensional problem to be treated directly in terms of Hermite tensor polynomials,[8] which is notationally more efficient than using the Hermite polynomials. For direct application involving the use of standard integrals the latter seem the best choice, and so we have used these throughout.

How is it we can apparently escape exercising the care suggested in Ref. 9 and plunge ahead, determining the c_n without considering the Hermitian adjoint equation? Specifically, why does Eq. (12) generate eigenfunctions that are orthogonal (with respect to the proper weight), so that these, rather than a biorthogonal set of eigenfunctions, provide the basis for an expansion? The reason for this seeming departure from normal procedure appears to be the explicit presence of the i in this equation, an unusual occurrence. Thus, in establishing the orthogonality properties of the ψ_n directly, if we multiply Eq. (12) by $\psi_m \exp(u^2 + 2k^2)$ and subtract from the equation with m and n interchanged, all goes well. However, if the biorthogonal set were required, we would multiply by $\psi_m{}^*$ times a weight function, and subtract the conjugated equation for ψ_m multiplied by ψ_n times the weight function. In the latter case the terms containing i do not vanish, leaving us without an orthogonality relationship for the conjugate pair.[7,8]

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Our debt to Ref. 9 for the basic insight into the problem considered here is most obvious throughout this paper, and we take this opportunity to explicitly acknowledge it.

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[7] One of us (S. H.) would like to thank Prof. N. Balazs for a stimulating discussion on this point.

[8] It is amusing to note that when the difficulties described in this paper are finally resolved and the results applied, the result given in a standard reference for one of the integrals commonly encountered is found to contain a misprint: In integral 7.374,7 of Ref. 11 the subscript on the Laguerre polynomial should be m, not n. In light of the other misprints we have mentioned, we consider this as strong evidence for the existence of Maxwell's demon!