1

Theoretical Framework underlying the Book

1.1 Introduction and the Essence of Our Approach

The purpose of this book is to develop and use an approach toward ecological phenomena constructed on the basis of certain methodologies inspired by physics and powered by various mathematical tools. The ecological phenomena of interest to us are typified by the spread of epidemics such as the Hantavirus as explained in Chapters 2–6, but also contain other subjects as found in Chapters 3–5 and 7–9 not involving the spread of diseases. It is the function of the present chapter to explain the essential ingredients of our theoretical approach and to provide an introduction to the mathematical tools that we use. We tend to the first task in this section and the next, and to the second task in the last two sections of the chapter. The description of the mathematic tools that we give could serve as an essential introduction for those who are not experts in their use but also as a focusing device for those who are.

Succinctly stated, our theoretical approach is based on the original conception of Newton in his study of physics and the developments of statistical mechanics carried out by Ehrenfest, Kac, and other prominent leaders (Uhlenbeck, 1955; Ehrenfest and Ehrenfest, 1959; Kac, 1959; Dresden, 1961) working in the field of mathematics applied to physical phenomena, and occasionally employs the techniques of nonlinear phenomena.

A central conception of Newton lay in assuming that every system is made of point particles whose motion (change of position with time) is responsible for *all* observations that could be made on the system. This was followed by Newton in understanding not only patently mechanical observations, i.e., ones associated with *motion* from a location to another, such as the movements of planets and projectiles, but also in describing unrelated branches of science like acoustics that dealt with sound, and optics that dealt with light. For instance, his corpuscular theory of light attempted to explain reflection and refraction in terms of forces acting on, and influencing the motion of, particles (corpuscles) of light as set out in his corpuscular

https://doi.org/10.1017/9781108882279.004 Published online by Cambridge University Press

theory of optics. It is not important to debate here whether Newton's conception can be said to have met with universal or partial success. What is significant is to realize that disciplines as varied as heat and materials science (the study of the properties of matter in the form of gases, liquids, and solids) were unified reasonably well in terms of his so-called kinematic plan of physics. Newton's major preoccupation was, thus, in regarding any given system as made up of constituent particles, understanding their motion, and deducing from that motion all desired information about the system.

Early forays into the analysis of ecological phenomena such as the spread of epidemics focused on relationships between properties of the system without space-differentiation. This was a bit as in thermodynamics where the behavior of a fluid may be described in terms of relations among a few variables such as the pressure, temperature, and volume. Space was introduced by many researchers (Okubo, 1980; Okubo and Levin, 2001; Murray, 2003a, 2003b) into the ecological considerations primarily as a feature added to thermodynamics-like studies to gain better accuracy in description. Our approach, on the other hand, is motion based right from the outset, in the spirit of the ambition of Newton's kinematic plan.

In our subject of ecology, we will consider *eco*-particles, which are nothing other than the animals whose motion and interactions we take as ultimately responsible for the observed eco-phenomena we will study. Let us assume there are N of them, label them by the numbers $i = 1$ to N, and call their respective positions in space $\boldsymbol{r}_i$. These are functions of the time t as the animals move. Time may be taken as continuous or discrete according to our preference and context of description. Under normal conditions the former would be our choice. However, if we want to emphasize a sequence of events that occurs after set intervals of time such as annually or at the beginning of each season, we might prefer to consider time to be discrete. Similarly, although space may be taken naturally continuous, dynamics on discrete lattices may also be studied, sometimes for mere numerical ease. Each animal may have internal observables, an example of which is the state of being infected or susceptible for infection; we will call the internal variable (or an array of variables) $\boldsymbol{\Omega}$. The state of the system at time t is, thus,

$$|\boldsymbol{\xi}(t)\rangle = |\boldsymbol{r}_1(t), \boldsymbol{\Omega}_1(t), \boldsymbol{r}_2(t), \boldsymbol{\Omega}_2(t), \ldots, \boldsymbol{r}_i(t), \boldsymbol{\Omega}_i(t), \ldots, \boldsymbol{r}_N(t), \boldsymbol{\Omega}_N(t)\rangle.$$

The dynamics of the system produces, from any given state $|\boldsymbol{\xi}'(t')\rangle$, a future state $|\boldsymbol{\xi}(t)\rangle$. This dynamics may be deterministic or probabilistic. Because our system is certainly not considered quantum mechanical at our highly macroscopic level of description, any probabilistic evolution would arise only from excluding a part of the underlying set of variables responsible for the dynamics from the time evolution explicitly. Probabilities also enter the description from two additional sources other than the dynamics. One of them, appropriate to any complex physical system, is the

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uncertainty in the specification of the initial state, which may be expressed via the Gibbs ensemble prescription (Gibbs, 1902). The other, peculiar to the fact that our system consists of animals, is that they may be considered to have free will in their actions. It is unnecessary for our purposes to enter into philosophical discussions on this account. From observation it is often clear that we may tackle this problem probabilistically. For these two reasons, we take as the primary state function of our system the probability (or probability density) $P_{\boldsymbol{\xi}}(t)$ that the system occupies state $|\boldsymbol{\xi}(t)\rangle$.

The two central questions then are how to calculate a given desired quantity from the probabilities, and how to determine the probabilities at a future time knowing them at a given earlier time. Because we have given the probabilities an ensemble interpretation from the point of view of the specification of the initial state, it is clear that the first question is to be answered through a linear operation (rather than something more exotic such as the bilinear prescription of quantum mechanics that is quite inappropriate at the ecological level of description). This is represented, for any observable that may be considered to be a function of the state as $O_{\boldsymbol{\xi}}$, via the prescription that the value of the observable is given by

$$\sum_{\boldsymbol{\xi}} O_{\boldsymbol{\xi}} P_{\boldsymbol{\xi}}(t), \tag{1.1}$$

where the summation over $\boldsymbol{\xi}$ represents integrations and summations appropriately according as the variable under question is continuous or discrete.

The other question, regarding the time evolution, is complex. In the context of Newton's classical mechanics, the state can be considered to be the Liouville density, which is a function of the positions and momenta of all the particles constituting the system, and the equation that governs the evolution can be taken to be the Liouville equation that involves Poisson brackets of the Liouville density with the Hamiltonian (Balescu, 1975; Reichl, 2009). As all students of mechanics know, there are other equivalent ways. In quantum mechanics, the state can be considered to be von Neumann's density matrix and the equation of motion the Liouville–von Neumann equation. It is usual in the study of the physics of macroscopic phenomena, as we are dealing with here, to take the governing equation to be the so-called Master equation

$$\frac{\mathrm{d}P_{\boldsymbol{\xi}}(t)}{\mathrm{d}t} = \sum_{\boldsymbol{\xi}'} \left[R_{\boldsymbol{\xi}\boldsymbol{\xi}'} P_{\boldsymbol{\xi}'}(t) - R_{\boldsymbol{\xi}'\boldsymbol{\xi}} P_{\boldsymbol{\xi}}(t) \right] \tag{1.2}$$

where the Rs are transition rates from state to state. Investigations of the origin of irreversibility around an intense period in almost precisely the middle of the twentieth century made it necessary (and/or useful) to augment the Master equation to include memory functions. Lucid presentations of the resulting governing

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equation, called from then on the generalized master equation (GME), are available in the work of several scientists, prominently Zwanzig (1964). The GME, which requires a description nonlocal in time, is particularly suited to represent motion with arbitrary degree of transport coherence and was put to detailed use in Kenkre and Knox (1974a), Kenkre (1977a), Kenkre and Reineker (1982). The GME has the form,

$$\frac{\mathrm{d}P_{\xi}(t)}{\mathrm{d}t} = \int_0^t dt' \sum_{\xi'} \left[\mathcal{W}_{\xi\xi'}(t-t')P_{\xi'}(t') - \mathcal{W}_{\xi'\xi}(t-t')P_{\xi}(t')\right], \tag{1.3}$$

and is sometimes augmented by a driving term. We will make do with the Master equation (1.2) in this book always at the uppermost, fully detailed, level of the ξ-states but will have occasion to use memory functions twice, in Chapters 8 and 9, to discuss coherent walks.

1.2 Description at Three Levels: Γ-space, μ-space, and Individual Models

Many systems, whether in physics or in ecology, consist, either solely or largely, of a collection of identical (or largely similar) particles, for instance, electrons, atoms, or animals. The question is often *how many* of them have a certain value for one of their properties, i.e., the occupation number of the particles (or eco-particles) in a particular state. This state is not $|\boldsymbol{\xi}\rangle$. Rather $|\boldsymbol{\xi}\rangle$ may be looked upon in part as the collection of the numbers in each *one-particle state*. If the system is thus constituted, and additionally if one's interest is only in properties that can be obtained in the fashion described from the numbers of particles (or eco-particles) in each one-particle state, it should be clear that an enormous simplification can be made in our description by restricting consideration to the one-particle space. This, as explained by the Ehrenfests in their discussions of statistical mechanics, is a descent from the original extremely complex space of $6N$ dimensions to one only of 6 dimensions. The number 6 is the number of spatial dimensions multiplied by 2 because Newton's equations are second order in time because positions and momenta are both free variables.

The original space of $6N$ dimensions was given the name Γ-space, while the reduced 6-dimensional space came to be known as the μ-space. The terminology was the Ehrenfests' (Ehrenfest and Ehrenfest, 1959, pp. 18 and 26). For our own considerations in our macroscopic pursuit of ecology, the respective number of dimensions is $3N$ for Γ-space and 3 for μ-space. This is so because of high damping in bio/eco systems (Berg, 1993). To appreciate the basic idea of this halving of the number of dimensions, consider Newton's equations of motion for a

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particle of mass m subject simultaneously to a potential $\mathcal{U}(\boldsymbol{x})$ and damping at rate γ,

$$m\frac{d^2\boldsymbol{x}}{dt} + \gamma\frac{d\boldsymbol{x}}{dt} + \nabla\mathcal{U}(\boldsymbol{x}) = 0. \tag{1.4}$$

If the damping γ is huge, as it is in the biological or ecological world, one may divide the above equation throughout by γ and write, to an excellent approximation,

$$\frac{d\boldsymbol{x}}{dt} + \nabla U(\boldsymbol{x}) = 0 \tag{1.5}$$

where $U(\boldsymbol{x})$ is $\mathcal{U}(\boldsymbol{x})/\gamma$, and the inertial term has been dropped because it is considered to be negligible. The order of the differential equation has changed during the passage from Newton's Eq. (1.4) to what we might call Aristotle's Eq. (1.5). The terminology we use stems from the fact that Aristotle stated that an object, if isolated, would remain stationary, whereas Newton made the brilliant discovery, incorporated famously in his first law of motion, that such an object would continue in its state of rest or of motion along a straight line. High damping is allowing us to ignore Newton's insight and, indeed, go back to Aristotle. Hence the halving of the order of the differential equation and consequently of the number of degrees of freedom. This is the Aristotelian (high damping) approximation that will underlie all our studies of the macroscopic ecological/biological world.[1]

All electrons are identical and so too all protons or all molecules of Helium. Mice, mosquitoes, birds, or bacteria, however, are *similar*, each within their class, but not identical, because there are minor variations between any two individuals. Treating them as identical is, however, a reasonable assumption for our purposes because of what we calculate. It behooves us, therefore, to formulate our theories in μ-space, whenever possible, rather than be plagued by the complexities of Γ-space. Our development of the theory of the Hantavirus, the West Nile virus, and of bacterial dynamics, in Chapters 2–5 will be, accordingly, in μ-space. In a section in Chapter 2, however, we will return to Γ-space considerations to perform computer simulations to explore what new insights we can thereby obtain in Hantavirus dynamics. We will also do that in most of Chapters 7 and 8 to aid our understanding of the formation of the dynamics of territories and flocks, respectively. And for the purposes of Chapter 6, we will quit μ-space in the other direction and perform model calculations on a system consisting of just two eco-particles, an infected rodent and an uninfected one. This will allow us to incorporate the minute detail demanded by separate home ranges of the two animals.

[1] We cannot resist drawing the reader's attention here to the sad spectacle of Mr. George Clooney receding tragically to isolation and death away from Ms. Sandra Bullock in outer space in the movie *Gravity* because of Newton's oppressive law. If the Aristotelian approximation (1.5) were fully valid, that tragedy would be avoided, and Mr. Clooney would be still among us.

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It is only rarely that the Master equation in Γ-space, Eq. (1.2), can be solved analytically. This is so because of the inherent complexity of the space. One of the uses of the Master equation is to deduce from it reduced equations in μ-space that might be more approachable. Direct solution of the original Master equation is nowadays often attempted via computer simulations. It is important to realize that the so-called Monte Carlo or cellular automata methods are simply solutions of the Master equation in full Γ-space, although nonanalytical, and to avoid misconceptions that they constitute independent theories.

Governing equations in μ-space, sometimes called kinetic equations, are typically derived from the top level of description provided by the Master equation in Γ-space. Yet, from a practical viewpoint, their predictions are not always precisely equivalent to predictions from the original Master equation. How can this be? The reason lies in the fact that, in deducing kinetic equations in μ-space, approximations must be perforce made. These can take the form of truncation of hierarchies, neglect of terms hoped to be small, replacement of expressions by more manageable ones, and similar procedures that are often ad hoc. This is the inevitable consequence of the enormous number of degrees of freedom and the ensuing complexity.

A case in point in standard nonequilibrium statistical mechanics, particularly in gas dynamics, is provided by the BBGKY hierarchy of reduced equations versus the Boltzmann equation (Balescu, 1975; Reichl, 2009). The latter can be regarded as obtained from the former by truncation, or by replacement of the connection to higher members of the hierarchy by nonlinear terms (the famous "collision terms") within μ-space. Another example is the problem of the validity of bilinear annihilation rates used in exciton phenomena when a reduced space description is employed (Kenkre, 1981).

The situation is that, although μ-space analysis should be equivalent to Γ-space analysis in principle, practically it never is fully so because of the various truncations, neglects, and approximations that are forced upon the investigator in her/his analysis. Ultimately, of course, the vindication of any theory employed must lie in its success (or failure) vis-à-vis observations. This is one of the reasons why, in this book, we keep to the tradition in physics of remaining close to experiment. We take rather seriously the task of maintaining a *continual dialogue* with field observations to steer our theoretical efforts. It is not enough to merely take an initial motivation from experiment and then barge merrily along one's analytic directions. One specific example of how our development of the theory relies on this dialogue with experiment is to be found in Chapters 5 and 6. Findings in the early part of Chapter 5 concerning home ranges are used to modify substantially our analysis as described in Chapter 6. Another instance is in the last section of Chapter 9, where such dialogue with experiment decides the type of nonlinearity to be used in the study of traveling waves of rodents.

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1.3 Theoretical Tools Used in the Book

In this section we discuss theoretical tools we have used in the book. We do so in a brief and introductory manner. Readers of different backgrounds and interests should employ them differently. We suggest that all glance at them rapidly. Then, if you are an expert at their use, use them only to whet your appetite and familiarize yourself with *our* notation and thrust. If you are on speaking terms with the tools but are not daily users of them, do study them to prepare yourself for what is to come in the main text in the book. If you know nothing about them, for instance, if you do not have a physics, mathematics, or similar background, we visualize a fork in the road. Either you should bite the bullet and start a serious study of the tools, or largely ignore them and read without their assistance. There is plenty in the main book that can be enjoyed and learned even without a detailed mastery of those theoretical tools.

The simplest manner to regard the motion of the animal, or creature such as a bacterium, in our words an eco-particle, is to treat it as performing a random walk. The justification for the random nature of the walk can come from a variety of sources, including even free will, but is primarily the large number of degrees of freedom we suppress in the description. If some special knowledge about the behavior of the eco-particle is available to us, we may inject it into the description, making the walk not totally random, but a self-avoiding walk, a Lévy flight or walk, a biased walk, or a walk correlated in other ways. We use in this book some of these and begin with the normal random walk.

1.3.1 Simple Random Walk and the Diffusion Equation

The simplest way of examining such a random walk is by imagining a one-dimensional ($1d$) lattice where the animal hops from a given site m to its right, i.e., to $m+1$, or to its left, i.e., to $m-1$. The number M_m of these animals, assumed noninteracting among themselves for this motion process, will change at the site m in the manner given by

$$\frac{dM_m}{dt} = F(M_{m+1} + M_{m-1} - 2M_m), \tag{1.6}$$

if we neglect overcrowding effects. Here F is the rate for the nearest-neighbor hop. A standard continuum limit, where the intersite distance l tends to zero, but F tends to infinity such that the product Fl^2 tends to a finite quantity, termed the diffusion constant D, turns Eq. (1.6) into the diffusion equation

$$\frac{\partial M(x,t)}{\partial t} = D\frac{\partial^2 M(x,t)}{\partial x^2}, \tag{1.7}$$

for the density $M(x,t)$, which is the limit of M_m/l as $l \to 0$.

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There are many other ways of deriving or understanding the diffusion equation (1.7), as, for example, from a combination of Fick's law and the continuity equation, but the above is most appropriate to this book.

To solve the equation for arbitrary initial conditions on the density, i.e., if $M(x,0)$ is known for all space, one Fourier transforms Eq. (1.7), solves the ordinary differential equation obeyed by the transform and inverts the result back into x-space. The well-known result is

$$M(x,t) = \int \Pi(x - x',t) M(x',0) dx', \tag{1.8}$$

where, for the infinite domain (in $1d$ for simplicity), the propagator is given by

$$\Pi(x,t) = \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}. \tag{1.9}$$

The propagator has Gaussian shape, but the solution can have arbitrarily complicated form depending on the initial density $M(x,0)$.

Needless to say, $M(x,t)$ may be understood not only as the density of noninteracting animals but also the probability density of a single individual. Let us interpret it in the latter manner for some of the following statements. A quantity often calculated for the random walker is the mean square displacement (MSD), which gives an indication of how far from an initial starting point the walker reaches on the average. Defined as

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 M(x,t) dx,$$

this (time-dependent) quantity is easily calculated from Eq. (1.9) and is found to increase linearly with respect to time t.

This result, usually attributed to Einstein, that the MSD equals the product of the time and the diffusion constant D of the walker, except for a known proportionality constant depending on the dimensionality, can be used simply to *measure* D because the MSD and the time are both measurable quantities.

1.3.2 Attracted Walk and the Smoluchowski Equation

Animals often are subject to attractor locations as they perform their random walks. An example is the existence of home ranges of rodents that roam on the terrain but return to specific "homes" that provide them with shelter and security. We will learn in the book how mutual attractive interactions, crucial to the process of flocking or herding, may also be regarded in terms of an attraction to a location in a multi animal higher space. Yet a third example is that the avoidance interaction in territorial animals can be cast as a movement of an individual within fluctuating (and

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confining) boundaries, whose separation distance is attracted toward a specified value. We will meet with these three examples in Chapters 6–8, respectively. How do we describe such walks, and what is the minimal mathematics necessary for the solution?

Let the random walker be simultaneously subjected to a potential $U(x)$ as it performs its random walk, and let us construct the potential to describe the attraction to a location, say the origin. The equation of motion would be

$$\frac{\partial M(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{dU(x)}{dx}M(x,t) + D(x)\frac{\partial M(x,t)}{\partial x}\right], \tag{1.10}$$

where we have allowed for the diffusion constant $D(x)$ to be generally space-dependent.[2] It is easy to work out the shape of the steady-state solution for the density by putting the time derivative equal to zero and solving the resulting ordinary differential equation in space. The shape is seen to be proportional to

$$\exp\left[-\int_{-\infty}^{x} dx' \frac{1}{D(x')}\frac{dU(x')}{dx'}\right].$$

The normalizing constant is trivially calculated. If D is constant, the shape is connected very simply to the potential:

$$e^{-U(x)/D}.$$

For the harmonic case $U(x) = (\gamma/2)x^2$ (linear restoring force), the steady-state shape is seen to be Gaussian, while a constant attractive force toward the origin with magnitude $\Upsilon|x|/x$, it is mod exponential. The time-dependent propagator for both these cases is also known. For the former, it is text book knowledge; for the latter, expressions appear to have been presented in the literature only recently by Touchette et al. (2010). A derivation of that propagator in both the time and the Laplace domain has been given independently also by Chase et al. (2016) using a quite different methodology and context. With $l = D/\Upsilon$, the propagator is

$$\begin{aligned}\Pi(x,x',t) = {} & \frac{1}{\sqrt{4\pi Dt}} e^{-\left[(x-x')^2+\Upsilon^2 t^2\right]/4Dt} e^{-(|x|-|x'|)/2l} \\ & + \frac{e^{-|x|/l}}{4l}\left[1 - \operatorname{erf}\left(\frac{|x|+|x'|-\Upsilon t}{\sqrt{4Dt}}\right)\right].\end{aligned} \tag{1.11}$$

The case of the harmonic potential has been known since the time of Smoluchowski himself. It is simpler in a way, perhaps even more physical than the other case because its restoring force varies with distance, and has been used in this book. The method of obtaining the propagator explicitly uses a Fourier transform

[2] Throughout the book, unless noted explicitly otherwise, D is to be considered to be constant.

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as in the case of the simple diffusion equation. However, it has to be followed by the solution of the first-order partial differential equation one gets in Fourier space by the method of characteristics. The result is essentially the one for the simple diffusion equation but with a *transformed time* $\mathcal{T}(t)$. The intriguing feature of this transformed time is that it is identical to the actual time t for short times but saturates to $1/2\gamma$ on the order of that time. This saturation leads to the characteristic Gaussian shape of the probability density at infinite time (rather than the uniform distribution that one obtains for the simple diffusion equation without an attractive center.)

At arbitrary times, the propagator of the Smoluchowski equation, wherein the random walker is pulled to the origin even as it is diffusing, is

$$\Pi(x, x', t) = \frac{e^{-\left(x - x' e^{-\gamma t}\right)^2 / 4D\mathcal{T}(t)}}{\sqrt{4\pi D\mathcal{T}(t)}}, \tag{1.12}$$

where the transformed time is given by

$$\mathcal{T}(t) = \frac{1 - e^{-2\gamma t}}{2\gamma}. \tag{1.13}$$

Notice the disappearance at rate γ of the effect of the initial position x' from which the walker starts, as displayed in the exponent of Eq. (1.12). Notice also the loss of translational invariance relative to the diffusion equation in that the propagator in Eq. (1.12) is not a function of $x - x'$.

1.3.3 Formalism for the Trapping of a Confined Random Walker

The analysis of several problems in our book has been facilitated by the application of the defect technique for the trapping of a confined random walker. Originated by Montroll and his collaborators (Montroll and Potts, 1955; Montroll, 1964, 1969; Montroll and West, 1979), the method has been used widely (Rubin and Weiss, 1982; Hughes, 1995; Redner, 2001). One example among many is to the area of the trapping and annihilation of Frenkel excitons moving in discrete lattices of molecular crystals (Kenkre, 1980; Kenkre and Reineker, 1982; Kenkre and Parris, 1983). A recent review with focus on motion in the continuum, and containing a number of novel results not available earlier, may be found in Spendier and Kenkre (2013).

Our interest in the present book is in a specialized situation not treated in most earlier uses of this defect formalism. It does concern a random walker that undergoes a reaction when it reaches a specific location but one that is simultaneously attracted to a center as described in the previous subsection. The location is generally different from the location of the attractive center. The reaction could consist

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of, for instance, being captured by a trap or annihilating something placed there or transmitting infection to an animal on encounter. This combined situation of confinement and trapping was developed by the authors of Spendier and Kenkre (2013) in collaboration with Sugaya in Spendier et al. (2013) and has been applied in this book in Chapter 6 to the transmission of infection in epidemics. As an introduction to the essential technique, we give its most simple trapping form below. It is relevant for a number of biological problems even outside ecology, such as funneling phenomena in photosynthesis (Clayton, 1980), DNA stretching with optical tweezers (Wang et al., 1997; Lindner et al., 2013), and electrostatic steering in enzyme ligand binding (Wade et al., 1998; Livesay et al., 2003).

Interpreting $M(x,t)$ as the probability density of the confined eco-particle (the random walking animal in the presence of an attractive center), we are generally interested in its survival probability

$$Q(t) = \int_{-\infty}^{+\infty} dx\, M(x,t) \tag{1.14}$$

when a term involving the capture parameter C_1 is appended to the Smoluchowski equation to represent capture of the eco-particle,

$$\frac{\partial M(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\gamma x M(x,t) + D\frac{\partial M(x,t)}{\partial x}\right) - C_1\delta(x-x_r)M(x,t), \tag{1.15}$$

$\delta(x-x_r)$ being a Dirac delta function representing the placement of a trap at $x = x_r$.

The defect technique leads to the solution in the Laplace domain. With ϵ denoting the Laplace variable and tildes denoting the Laplace transform, if the initial condition of the particle placement is localized at a single point x_0, the survival probability is given in terms of the (Laplace transforms of the) propagators of the Smoluchowski equation, which we know from Eq. (1.12):

$$\widetilde{Q}(\epsilon) = \frac{1}{\epsilon}\left[1 - \left(\frac{\widetilde{\Pi}(x_r,x_0)}{(1/C_1) + \widetilde{\Pi}(x_r,x_r)}\right)\right]. \tag{1.16}$$

Because the propagators are known in the time domain but their transforms are not known analytically in the Laplace domain, much of the subsequent analysis has to be done numerically. Some of that study has been worked out analytically, however, for the case of the constant force (potential linear in the coordinate rather than quadratic) by Chase et al. (2016). We refer the reader for further details of this development of the trapping of a confined random walker to Spendier et al. (2013) and Chase et al. (2016), and for a more complete account of the general problem of the defect technique in continuum space to Spendier and Kenkre (2013).

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Useful background material for motion on discrete lattices may be found in the early papers by Lakatos-Lindenberg et al. (1972) and Kenkre and Wong (1981) and a recent one by Giuggioli (2020). In Chapter 6 it will be shown how the trapping analysis is generalized to the problem of infection transmission.

1.3.4 Memory Functions and the Telegrapher's Equation for Partially Coherent Transport

Among the bewildering variety of time evolutions found in nature, two can be identified as extreme limits: oscillations and decays. How memory functions unify these two limits has been explained elsewhere (Kenkre, 2003) in contexts as varied as sensitized luminescence and compaction of granular materials (Kenkre et al., 1998; Scott et al., 1998; Kenkre, 2001a, 2001b). Memory functions appear both naturally in the derivation of the Master equation from the very microscopic starting point (Zwanzig, 1964) and more pragmatically at coarser levels of description as a device to incorporate coherence in motion (e.g., Kenkre, 1974). The interested reader is referred to a book whose entire first half was devoted to this task in the context of the motion of Frenkel excitons (Kenkre and Reineker, 1982). Here we draw attention first to the fact that coherence can be incorporated as an added feature to random walks by augmenting the diffusion equation, Eq. (1.7), through a memory function $\phi(t)$,

$$\frac{\partial M(x,t)}{\partial t} = D \int_0^t dt' \phi(t-t') \frac{\partial^2 M(x,t')}{\partial x^2}. \tag{1.17}$$

If $\phi(t)$ decays infinitely fast, i.e., is a Dirac delta-function, Eq. (1.17) becomes the diffusion equation (1.7), whereas if $\phi(t) = 1$, i.e., is constant for all time, a time differentiation shows that we get a wave equation. An intermediate memory typically gives wave behavior at short times and diffusive behavior at long times. Specifically, if $\phi(t) = \alpha e^{-\alpha t}$ and $c^2 = D\alpha$, Eq. (1.17) yields, on differentiation with respect to time,

$$\frac{\partial^2 M(x,t)}{\partial t^2} + \alpha \frac{\partial M(x,t)}{\partial t} = c^2 \frac{\partial^2 M(x,t)}{\partial x^2}. \tag{1.18}$$

Here c is the speed of the wave in the "coherent" limit $\alpha \to 0$. This so-called *telegrapher*'s equation has an ancient heritage since the time of Heaviside and Lord Kelvin and produces an intricate joining of wavelike (coherent) propagation with diffusive (incoherent) motion: in extreme parameter limits as well as in time for given parameter values. Coherent motion at short times becomes incoherent at

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sufficiently long times in this case. Indeed, for initial localization at the origin, the mean square displacement (MSD) from the telegrapher's equation (1.18) goes as t^2 at short times, as t at long enough times, and at all times is expressed as

$$\langle x^2 \rangle = 2D\left(t - \frac{1 - e^{-\alpha t}}{\alpha}\right). \tag{1.19}$$

This is an expression that bridges the two limits in a natural and smooth manner. While the concept is straightforward enough that it must have been used independently by many, an early instance we are familiar with, particularly in the context of a specific application to experiment, is in Kenkre (1974). Indeed, Eq. (1.19) was used to construct a theory of fast and slow transfer rates of Frenkel excitations almost half a century ago (Kenkre and Knox, 1974b). A prescription was also given (Kenkre and Knox, 1974a) for calculating the memory functions from microscopics, generalizing the venerable Förster theory of excitation transfer employed in photosynthesis and sensitized luminescence (Förster, 1948).

More exotic memories, e.g., algebraic, yield exotic behavior, e.g., power dependences. A direct relationship between the mean square displacement (MSD) and (arbitrary) memory in Eq. (1.17) is available for the localized initial condition mentioned above as

$$\langle x^2 \rangle = D\int_0^t dt' \int_0^{t'} dt'' \phi(t''). \tag{1.20}$$

It was this double integral connection (Kenkre and Knox, 1974b; Kenkre, 1977a) that was at the heart of a clean natural resolution of the so-called R^3 versus R^6 Perrin–Förster puzzle in the theory of luminescence.

There are many microscopic sources of such memory functions, some arising from the quantum dynamics of the system and some purely classically simply from coarse-graining of the description. One entertaining example is a "railway track model" described in Kenkre and Sevilla (2007), which is built on the simple picture of a classical particle moving unimpeded at speed c for variable lengths (whose average is the mean free path) and then getting scattered in times of the order of $1/\alpha$. The motion is wavelike for traversal distances shorter than the mean free path but diffusive at times longer than the scattering time $1/\alpha$.

The exponential memory function, associated with the telegrapher's equation, has been used to introduce motion coherence into the nonlinear Fisher equation for the analysis of traveling waves (Manne et al., 2000; Abramson et al., 2001, 2002) and also for the inclusion of similar effects in territorial dynamics (Giuggioli et al., 2012; Sarvaharman et al., 2019). The description will be found, respectively, in Chapters 8 and 9 of this book.

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1.3.5 Nonlinear Equations and Simple Tools for Their Analysis

Central to the theoretical description in the book are nonlinear partial differential equations constructed by adding an appropriate term to the diffusion equation (1.7). The added term, nonlinear in the density of the eco-particles (the animals) refers to supporting processes other than motion: birth, death, and competition. The most used is the logistic term, and the result is the well-known Fisher–Kolmogorov–Petrovsky–Piskunov equation, called in this book the Fisher equation for brevity (Fisher, 1937; Kolmogorov et al., 1937):

$$\frac{\partial M}{\partial t} = D\frac{\partial^2 M}{\partial x^2} + C_1 M(C_2 - M), \tag{1.21}$$

where the C's are constants. In a part of our analysis we incorporate the so-called Allee effect and replace the (quadratic) logistic term by a cubic term to obtain the Nagumo equation,

$$\frac{\partial M}{\partial t} = D\frac{\partial^2 M}{\partial x^2} + C_1 M(C_2 - M)(M - C_3), \tag{1.22}$$

containing three constants, including C_3. We also study variants of these equations, which describe long-range competition.

Nonlinearity makes these partial differential equations insoluble analytically and forces one to employ standard numerical methods. Of use are also well-known procedures of nonlinear science including linear stability and bifurcation investigations. Putting all derivatives to zero yields fixed points, which are the solutions that are independent of time and space. Inspecting small departures from these fixed points and keeping only linear terms in the evolution allows the determination of spectra and the understanding of patterns. These standard features of nonlinear science are explained thoroughly in a number of modern books, including in particular Nicolis (1995) and Strogatz (2018).

1.3.6 Convective Motion and Related Methods

Consider the logistic term in the Fisher equation above replaced by an arbitrary nonlinearity represented by $F(M)$ and the diffusive term replaced by a convective counterpart. The result is

$$\frac{\partial M}{\partial t} + v\frac{\partial M}{\partial x} = F(M), \tag{1.23}$$

where v denotes the velocity with which the individual eco-particles move convectively instead of diffusively.

A prescription for obtaining exact solutions is straightforward, was given in Kenkre (2004), and was put to use by the authors of the present book (Giuggioli

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and Kenkre, 2003) in collaboration with Peixoto et al. (2005). The prescription is as follows. One introduces a function $g(M)$ through

$$\frac{dg}{dM} = \frac{1}{F(M)}, \tag{1.24}$$

rewrites the nonlinear partial differential equation for $M(x,t)$ in terms of a *linear* counterpart for $g(x,t)$, finds the explicit solution of the latter for the initial value problem as[3]

$$g(x,t) = g\left(M_0(x - vt)\right) + t, \tag{1.25}$$

where $M_0(x)$ is the spatial distribution $M(x,0)$ at the initial time, and finally converts $g(x,t)$ into a solution for $M(x,t)$ by applying the inverse of the function g:

$$M(x,t) = g^{-1}\left[g\left(M_0(x - vt)\right) + t\right]. \tag{1.26}$$

Here is an illustration of the technique. Consider the Fisher-like equation with the quadratic nonlinearity so that $F(M) = AM - BM^2$. The above procedure yields

$$g(M) = \ln\left[\left(\left|1 - \frac{A/B}{M}\right|\right)^{-1/A}\right],$$

which leads to the exact solution

$$M(x,t) = \frac{1}{\frac{e^{-At}}{M_0(x-vt)} + \frac{B}{A}(1 - e^{-At})}. \tag{1.27}$$

This solution has been extensively studied in Giuggioli and Kenkre (2003).

Consider now the Nagumo-like equation with the cubic nonlinearity as given in the previous section. Now $F(M) = -BM(M-H)(M-C)$. If the last factor were absent, this would correspond to $H = A/B$ in the previous paragraph relating to the Fisher-like equation. For this case,

$$g(M) = -(1/B)\ln\left[M^{1/HC}(M - C)^{-1/[C(H-C)]}(M - H)^{1/[H(H-C)]}\right],$$

where it should be noted that M is $M(x,t)$, a function of space and time, while B, C, and H are constants. The solution for $M = M(x,t)$ in terms of the initial dependence $M_0 = M(x,0)$ is obtained, analytically but implicitly, as (Kenkre, 2004)

$$\begin{aligned} &M(x,t)^{1/HC}[M(x,t) - C]^{-R/C}[M(x,t) - H]^{R/H} = e^{-Bt} \\ &M_0(x - vt)^{1/HC}[M_0(x - vt) - C]^{-R/C}[M_0(x - vt) - H]^{R/H}, \end{aligned} \tag{1.28}$$

[3] In the original publication (Kenkre, 2004), $g(M)$ was defined with a minus sign and therefore resulted in the counterpart of the prescription (1.25) having $-t$ rather than $+t$ as here. The two are obviously equivalent.

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where $R = 1/(H - C)$. Note that the solution $M(x,t)$ appears in the left-hand side of the equation, whereas the initial density $M(x,0)$ is called $M_0(x)$ and boosted as $M_0(x - vt)$ in the right-hand side. This method will be found used in Chapter 9.

Finally, a related procedure that we will mention in Chapter 8 to study herding or flocking is described briefly. Let us consider again a first-order nonlinear partial differential equation (without a diffusive term), but let the nonlinearity consist not of an additive dependence on the density as in Eq. (1.23) but, instead, in what appears as a spatially dependent velocity:

$$\frac{\partial M(x,t)}{\partial t} = \frac{\partial \left[F(x)M(x,t)\right]}{\partial x}. \tag{1.29}$$

Here, $F(x)$ is an arbitrarily nonlinear function of the coordinate x and represents a velocity of the eco-particle moving right. If we multiply throughout by $F(x)$ and define a new variable G via

$$\frac{dG}{dx} = \frac{1}{F(x)}, \tag{1.30}$$

we get a simple convective equation in G-space for the quantity $N(G,t) = F(x)M(x,t)$, which is solved as

$$N(G,t) = N_0(G + t),$$

where $N_0(G) = F(x)M(x,0)$. This means that the solution for any initial distribution $M(x,0)$, which we will call $M_0(x)$, is given by

$$M(x,t) = \frac{F(G^{-1}[G(x) + t])}{F(x)} M_0\left(G^{-1}[G(x) + t]\right). \tag{1.31}$$

The steps to use the procedure are (i) calculating $G(x)$ from the integration of $1/F(x)$, (ii) obtaining explicitly the inverse G^{-1} so that x can be expressed as a function of G, and (iii) starting from the initial condition $M(x,0)$, writing down the solution as Eq. (1.31).

Here is a simple example. Let $F(x) = \gamma x$ so that Eq. (1.29) is the Smoluchowski equation with quadratic potential but without diffusion.

Step (i): Evaluation of the integral gives $G(x) = (1/\gamma) \ln x$.

Step (ii): Inversion is explicit as $x = \exp(\gamma G)$.

Step (iii): The solution for arbitrary initial condition is

$$M(x,t) = e^{\gamma t} M_0(x e^{\gamma t}). \tag{1.32}$$

An application will be found in Section 8.2.5.

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1.3.7 Langevin Approach and the Fokker–Planck Equation

One last comment about our theoretical framework. The μ-space or Γ-space methodology discussed at the beginning of this chapter is like an aerial view of the system. There is another way of developing the theory, which is known as the Langevin approach, which we do not explicitly use in the book. That approach arises from what is called a Brownian motion analysis and consists of focusing in full detail on a small part of the complete system, treating the rest (often called the reservoir), in a more blurry fashion. In contrast with the aerial view we have been discussing above, the Langevin approach is based on the view of an infantry unit down on the ground. Only the immediate neighborhood is considered in full detail, and information about (conceptually) more distant parts of the environment are relegated to the status of a reservoir.

The reservoir provides "noise," by which is meant "random" or "stochastic" terms in the evolution of the subsystem one has chosen to focus on. Two practical approaches to the descriptions of systems in the presence of noise exist. One considers the evolution in the presence of a mix of stochastic and systematic terms, the latter treated in full detail and the former in only a simple rudimentary way that attempts to capture the essential ingredients of the interaction with the reservoir. The resulting (often ordinary) differential equations are termed stochastic differential equations. The other, equivalent, approach, which we happen to prefer to use in this book, focuses on the probabilities (or probability densities) that the observables of the subsystem have given values. These probability densities obey partial differential equations said to be the Fokker–Planck equation for that particular problem. There is nothing stochastic in the solution of such a Fokker–Planck equation. Simply from being what they are, and from the prescription through which they predict expectation values of the observables, the probabilities themselves bring in the stochastic element.

Thus, the diffusion equation (1.7) is the Fokker–Planck equation for the Langevin equation

$$\frac{dx}{dt} = R(t), \tag{1.33}$$

provided the noise $R(t)$ is "white," which means delta-correlated in time, has zero mean, and is Gaussian with strength determined in the standard way by the diffusion constant D. The Smoluchowski equation (1.10) for the case of the harmonic potential is the Fokker–Planck equation for the Langevin equation

$$\frac{dx}{dt} = -\gamma x + R(t), \tag{1.34}$$

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if similar conditions are satisfied by the stochastic noise $R(t)$. These two are, respectively, referred to as a Wiener process and an Ornstein–Uhlenbeck process.

It is often said that the Langevin approach and the Fokker–Planck approach promote, respectively, a Lagrangian and an Eulerian picture, the latter terms referring to fluid dynamics. Others compare the two to the Heisenberg and the Schrödinger pictures in quantum mechanics. Two excellent sources for the practical methodology are Risken (1984) and Wax (1954).

1.4 Useful Theoretical Tools Not Used in the Book

The theoretical tools described in the previous section have been used throughout this book, and familiarity with them will be of help to the reader for an understanding of the analysis in the book. We also want to mention that "extra" techniques are available to the researcher who wishes to extend the studies described in novel directions. Such additional techniques include those that have been spawned by the famous paper by Montroll and Weiss (1965) on the continuous time random walk (CTRW), those related to recent activity based on fractional diffusion equations (FDE) since the work by Schneider and Wyss (1989), and those related to the well-known Lévy walk (Shlesinger et al., 1986; Shlesinger and Klafter, 1986; Zaburdaev et al., 2015).

Examples of the first, i.e., of the CTRW, can be found in Bel and Barkai (2005), Grigolini (2006), and Metzler et al. (2014). Some examples of the FDE studies are in Saichev and Zaslavsky (1997), Podlubny (1999), Metzler and Klafter (2000), Mainardi et al. (2001), and West et al. (2003). And examples of applications to animal ecology of non-Brownian walk methods (Shlesinger et al., 1982) are in Viswanathan et al. (2011) and associated with the long-standing debate about the so-called Lévy foraging hypothesis (Viswanathan et al., 1999; Bartumeus et al., 2005; Benhamou, 2007; Edwards, 2011; Reynolds, 2015; Pyke, 2015).

The analysis of tracking data through concepts such as Hurst exponents (Hurst et al., 1965) and multifractality (Kantelhardt et al., 2002; Seuront and Stanley, 2014) has pushed forward novel methods to analyze movement statistics (Barabási and Stanley, 1995; Giuggioli et al., 2007; Kumar et al., 2009a) and brought to the fore techniques to extract power law exponents from animal displacements (Giuggioli and Bartumeus, 2010; Bartumeus et al., 2010; Giuggioli and Bartumeus, 2012). Other complex walks include fractional Brownian motion (Mandelbrot and Van Ness, 1968; Biagini et al., 2010) and self-avoiding walks (Madras and Slade, 2013). The latter might be used to represent animals that tend not to return to where they have once been for foraging because food might be scarce after it was consumed.

The task of determining the relationships that some of these formalisms bear to one another is obviously important to the community of investigators. This includes, notably, the GME-CTRW equivalence (Kenkre et al., 1973; Kenkre and Knox, 1974a; Kenkre, 1977a), the FDE-CTRW connection (Hilfer and Anton, 1995), and the GME-FDE equivalence (Barkai et al., 2000; Giuggioli et al., 2009). The relation between these three formalisms and one in which transport coefficients such as the diffusion constant have a time dependence, has also been investigated explicitly (Kenkre, 2001a; Kenkre and Sevilla, 2007). These relationships are presented in some detail at the end of this book in Appendix A.

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