1
Introduction

1.1
Overview of Nonlinear Wave Phenomena

Examples of nonlinear wave phenomena abound in the physical, biological, and social sciences. One of the most striking instances is the solitary wave in shallow water in a narrow channel. In 1844, the Scottish naval engineer, John Scott Russell recalled an event some 10 years prior in which he observed a single humped wave (which he called a "wave of translation") that preserved its shape over a great distance as he followed it on horseback, arguably the first reported experimental observation of a nonlinear solitary wave [1]. The wave he observed had a height of about 0.3 m and a width of about 10 m, and was created by the sudden stopping of a barge in a narrow canal. He was so clearly struck by this observation that he described this experience as his "first chance interview with that singular and beautiful phenomenon". Initial attempts to explain this remarkable phenomena using approaches based on the then well-known linear wave equation failed. While Boussinesq and Lord Rayleigh made considerable theoretical progress in the 1870s, it was not until 1895 (and some 50 years after Russell's intitial experimental report) with the treatment of the Korteweg–de Vries (KdV) nonlinear wave equation, that the solitary shallow water wave received its conclusive explanation [2]. The KdV equation can be written in the form:

$$2\frac{\partial \psi}{\partial t} + 3\psi \frac{\partial \psi}{\partial x} + \frac{1}{3}\frac{\partial^3 \psi}{\partial x^3} = 0\,, \tag{1.1}$$

where $\psi(x,t)$ denotes the height of the fluid surface at position x along a straight narrow channel, and t denotes time. Take note of the presence of the quadratic nonlinearity in the second term. This equation can be derived from basic laws of fluid dynamics. One finds a family of single-humped solutions to this equation that move *without dispersing*. Furthermore, one finds that *the speed of the wave is dependent on its amplitude*. Both of these properties cannot be captured by using a standard linear wave equation. For instance, an initial shape in the solitary wave form is made up of several wavelengths and must, therefore, quickly disperse and devolve into its constituent modes.

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Another more recent example, and one with which many are familiar, is the dynamics of traffic flow, including the causes of traffic jams. One can construct a simple and remarkably descriptive nonlinear wave model with the following two simple ingredients: 1) the law of "mass" conservation, in this case car conservation, which can be written for one lane of traffic flow in the following one- dimensional form as

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0\,, \tag{1.2}$$

where $\rho(x,t)$ denotes the number of cars per unit length at space-time point (x,t), and $j(x,t)$ denotes the rate at which the cars pass the point x per unit time at time t, in other words, the vehicle "current"; and 2) a constitutive relationship between j and ρ, which takes the form $j = \int v(\rho)\, d\rho$ where $v(\rho)$, denotes the *density-dependent* velocity of the vehicles, which may be obtained by empirical observation [3]. Clearly, if the density is very high, everyone drives more slowly and at some point of high enough density, the average velocity tends to zero. Incorporating this density-dependent velocity into the vehicle conservation equation gives rise to a nonlinear wave equation of the following form:

$$\frac{\partial \rho}{\partial t} + v(\rho)\frac{\partial \rho}{\partial x} = 0\,. \tag{1.3}$$

Among other things, this equation reveals *shock wave* solutions moving at a precise speed and in which the density jumps discontinuously between relatively high and low values for a wide class of functional forms for $v(\rho)$. If a diffusive term is added in the right hand side of Eq. (1.3), the discontinuity in the shock wave is somewhat smoothed: the wave profile has a steep gradient in a narrow region whose width is determined by the diffusion coefficient. This system illustrates yet another feature of nonlinear wave systems that are not possible to find in solutions of a linear wave equation, namely, shock-like boundary layers between well-defined values with a shape that exhibits no dispersion as the shock moves through its medium.

A prominent example from biology concerns the propagation of nerve impulses in humans and animals. The effective transmission line in this case is the axon and the wave is of an electrochemical nature involving the lateral diffusion of ions across the membrane boundary of the axon. This type of nonlinear wave can be described by the following set of equations known as the FitzHugh–Nagumo model [4, 5]:

$$\frac{dU}{dt} = f(U) - W + I + D\frac{\partial^2 U}{\partial x^2}\,, \tag{1.4}$$

$$\frac{dW}{dt} = U - B\,W\,, \tag{1.5}$$

where $U(x,t)$ corresponds to the lateral electric potential across the axon membrane, $f(U)$ is a nonlinear function which describes regenerative self-excitation in the system, $W(x,t)$ corresponds to an outward-flowing ion current, I denotes a stimulus current, D is an effective diffusion constant for the membrane potential, and B is a constant. The solutions of this system exhibit several features associat-

ed with nerve pulses, for example, a traveling solitary wave structure in which the waves have a particular amplitude, time-dependence of the variables that typically possess regions of rapid and then gradual change which suggests the role of *multiple time scales*, and refractory behavior in which there is a certain period of time during which it is not possible to excite the medium. It should also be noted that none of these features is captured by a linear wave equation approach.

Chemical reactions provide yet another example. There is a class of autocatalytic chemical reactions (e. g., Belousov–Zhabotinsky reaction) which show temporal oscillatory behavior in the constituent molecular concentrations when they are well-stirred in order to keep them spatially homogeneous [6]. When they are not stirred, these same systems can show propagating spiral wave patterns of great complexity. This behavior can be modeled by a reaction-diffusion system:

$$\frac{\partial n_i}{\partial t} = \nabla \cdot (D \nabla n_i) + R_i(\{n_j\}) \,, \tag{1.6}$$

where the $n_i(r, t)$ (with $i = 1, 2, \ldots, N$) denote the space and time-dependent concentrations of different molecular species in the reacting mixture, and R_i is the reaction rate for the i-th species. Typically, R_i is a nonlinear function of the concentrations because the reactions involve two or more molecules per reaction. For example, in a simple binary reaction of the form $\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C}$, the corresponding reaction rate R_C for species C includes a term that is proportional to $n_\mathrm{A} n_\mathrm{B}$ according to the mass action law. For specific reactions, this system exhibits nonlinear spiral waves in two spatial dimensions. If one neglects the reaction term, one has the usual linear diffusion equation and thus, the underlying parabolic partial differential equation is very different than the wave equation. The reaction terms may give rise to *bistability* of two different time-independent solutions, another common feature that distinguishes nonlinear from linear wave phenomena.

In this book, we will focus on the development and application of nonlinear wave methods for problems involving the transport of electric charge in solid materials. The realization that nonlinear charge waves occur in condensed matter is relatively young and is largely traceable back to the discovery of the Gunn effect in GaAs in the early 1960s [7]. In a seminal paper, Gunn found that when doped GaAs samples were subjected to sufficiently high voltage, they emitted strong microwave radiation. He subsequently verified in a series of capacitive probe measurements that the microwave radiation was due to periodically cycling domains of high electric field propagating along the samples in the direction of current flow. In the next section, we review the basics of classical charge transport in solid media and point out, in simple terms, where it is that the crucial nonlinearities may arise.

1.2
Nonlinear Waves and Electronic Transport in Materials

Here, we review the essentials of electronic transport in solids at a level similar to that of a typical undergrad course in electricity and magnetism. We also introduce

the drift-diffusion form of electrical current. We start by recalling that conservation of charge is expressed by the following well-known continuity equation

$$\nabla \cdot \boldsymbol{j} + \frac{\partial \rho}{\partial t} = 0 \,, \tag{1.7}$$

where $\boldsymbol{j}$ now denotes the three-dimensional *electrical current density* (SI units are $\mathrm{A/m^2}$) and $\rho(\boldsymbol{r}, t)$ denotes the three-dimensional charge density. We also have the basic electrostatic relationship between electric field and charge density, one of the Maxwell equations expressed as

$$\nabla \cdot \boldsymbol{E} = \frac{\rho(\boldsymbol{r}, t)}{\kappa \epsilon_0} \,. \tag{1.8}$$

Finally, we have a constitutive relation between the electric field and current density that flows in the material. The simplest and most common assumption is the local version of Ohm's law,

$$\boldsymbol{j} = \sigma \boldsymbol{E} \,, \tag{1.9}$$

that is, a linear proportionality between the applied electric field and the current that flows, where σ denotes the electrical conductivity. Even though this is an empirical relationship, it works quite well for many materials and applications. It can be derived in a number of ways, from the elementary Drude argument to sophisticated quantum mechanical calculations that take full account of energy band structure and scattering mechanisms [8, 9].

Let us briefly recall the Drude form of the dc conductivity,

$$\sigma = \frac{n e^2 \tau}{m^*} \,, \tag{1.10}$$

where n denotes the volume density of mobile charge carriers (e. g., electrons), e is the electron charge, m^* is the effective mass of the charge carrier in the material of interest [8], and τ denotes the scattering time. In both semiconductors and metals, the mobile charge carriers (electrons and/or holes) are compensated by a background of fixed charge (associated with ionic constituent atoms of the underlying crystal lattice) of opposite sign. If we denote the density of these fixed charges by N, then we have for total charge density the following relationship:

$$\rho(\boldsymbol{r}, t) = e\,(n(\boldsymbol{r}, t) - N) \,, \tag{1.11}$$

where we have assumed that n can vary in space, but that N is constant.

If we now combine Poisson's Law and Ohm's Law, Eqs. (1.8) and (1.9), respectively, we have:

$$\nabla \cdot \boldsymbol{j} = \sigma \nabla \cdot \boldsymbol{E} = \frac{\sigma}{\kappa \epsilon_0} \rho(\boldsymbol{r}) \,. \tag{1.12}$$

This equation can be brought into a form depending only on $\rho(\boldsymbol{r}, t)$ by using the charge continuity equation (1.7)

$$\frac{\partial \rho}{\partial t} = -\frac{\sigma}{\kappa \epsilon_0} \rho(\boldsymbol{r}, t) \equiv -\frac{\rho(\boldsymbol{r}, t)}{\tau_d} \,, \tag{1.13}$$

where we have defined the *dielectric relaxation time*: $\tau_d \equiv \kappa\epsilon_0/\sigma$. Equation (1.13) is often referred to as the dielectric relaxation equation. Imagine an initial condition in which the charge density at a point $\boldsymbol{r}$ has a value $\rho_0 \neq 0$ which might occur due to a thermal fluctuation or a rapid voltage pulse applied to the system. Then at subsequent times, the charge density decays exponentially to zero as mobile charges from other parts of the material flow into the region at point $\boldsymbol{r}$ to neutralize the overall charge density

$$\rho(\boldsymbol{r}, t) = \rho_0 \exp\left[-\frac{t}{\tau_d}\right] . \tag{1.14}$$

This result leads to the immediate conclusion that we do *not* expect to find nonlinear charge waves in transport systems that are well-described by Ohm's Law; the state in which $\rho \to 0$ in the interior of a homogeneous material is always stable. However, Eq. (1.14) does yield an additional insight, namely, that instability might occur if the conductivity σ were somehow negative. Referring back to the elementary dc conductivity expression, Eq. (1.10), we can see that this is unlikely since the constituent's parameters are all positive. However, if we allow for a nonlinear constitutive relationship between current density and applied field, we can recognize the possibility to achieve a *differential* conductivity that is negative for a certain range of field values. This book is largely centered on such systems in nature.

Returning to Ohm's Law, cf. Eq. (1.9), we note that it can be written in the form $j = env$ where v denotes the drift velocity, that is, the average velocity of all the carriers in an applied electric field E. Regarding the Ohm's Law case, it is stated that $v = e\tau E/m^*$, that is, a linear relationship between drift velocity and applied field. We can generalize this to consider a nonlinear dependence of drift velocity on field which we denote by $v(E)$. Additionally, a study of statistical transport theories shows that, in general, the current will take the form of a gradient expansion in the density of the mobile charges [10, 11]. If we restrict ourselves to only one spatial dimension (call it the x-direction), j_x can be expanded in a series of terms proportional to $\partial^i n/\partial x^i$. For charge transport problems (even nonlinear ones), it generally suffices to retain the first two terms of such an expansion (i. e., $i = 0$ and 1) which gives the drift-diffusion expression for current density:

$$j_x = e\left[nv(E) - D(E)\frac{\partial n}{\partial x}\right] , \tag{1.15}$$

where $D(E)$ denotes the (possibly field-dependent) diffusion constant for the charge carriers. Let us now repeat the above steps that previously lead to the dielectric relaxation equation, though now using the drift-diffusion form of the current. Firstly, we note that we use the Poisson equation to write the charge continuity equation in the form

$$\frac{\partial j_x}{\partial x} + \kappa\epsilon_0 \frac{\partial^2 E}{\partial x \partial t} = 0 , \tag{1.16}$$

which can be immediately integrated with respect to x to yield

$$j_x + \kappa\epsilon_0 \frac{\partial E}{\partial t} = J(t) . \tag{1.17}$$

In this form of Ampère's law, the total current density $J(t)$ is the sum of the electrical current density j_x and the displacement current $\kappa\epsilon_0\partial E/\partial t$. Multiplied by the cross section, it denotes the boundary current that flows into and out of the structure. At this point, we replace the current density j_x by the drift-diffusion expression to write:

$$env(E) - eD(E)\frac{\partial n}{\partial x} + \kappa\epsilon_0\frac{\partial E}{\partial t} = J(t)\,. \tag{1.18}$$

However, this equation involves both variables n and E, and it is desirable to write a dynamical equation entirely in terms of one of these. We can eliminate n in favor of E using the Poisson Equation, cf. Eq. (1.8), and also recalling the relationship between n and ρ, cf. Eq. (1.11):

$$\frac{\partial E}{\partial t} + v(E)\frac{\partial E}{\partial x} - D(E)\frac{\partial^2 E}{\partial x^2} = \frac{J(t) - eNv(E)}{\kappa\epsilon_0}\,. \tag{1.19}$$

We can immediately see a qualitative analogy with the traffic flow equation, cf. Eq. (1.3). The field-dependent drift velocity of carriers is analogous to the density-dependent vehicle velocity. For appropriately shaped $v(E)$, one may also expect the formation of shock waves. Additionally, we have diffusion and source terms to consider that are similar in form to those in the first equation from the FitzHugh–Nagumo model, cf. Eq. (1.4). Therefore, we may also expect to see oscillatory and excitatory behavior that is reminiscent of nerve propagation. As we shall see, Eq. (1.19) forms the basis of an effective model of the Gunn effect studied in Chapter 6.

Another way in which nonlinearity may enter into the charge transport picture in a very basic and widespread manner is through the inclusion of trapping dynamics, whereby the mobile charge carriers may become trapped and liberated from trapping sites. This will be discussed in detail in Chapter 7, and thus, we mention only the simplest aspect of this behavior here. Let $n_t(\boldsymbol{r}, t)$ denote the density of charge carriers that are trapped on trapping sites. If the total density of traps is N, then the local charge density should be written as $\rho(\boldsymbol{r}, t) = e\,(n(\boldsymbol{r}, t) + n_t(\boldsymbol{r}, t) - N)$. Let us consider the form of local rate equation for the n_t. Clearly, n_t will be increased when a free charge carrier is trapped on an available site, a process known as *capture*. This process must be proportional to the density of free carriers and the density of available sites, that is, proportional to the product $n(N - n_t)$. Similarly, we expect n_t to decrease due to excitation of trapped charge carriers, for example, by external illumination of an appropriate frequency or by the absorption of energy from other excitations in the material, for example, phonons [8]. This process is known as *generation* and is only proportional to the density of trapped charges n_t. Another process that decreases n_t occurs when a sufficiently energetic free carrier collides with a trap carrier and imparts sufficient energy to liberate it. This process is known as *impact ionization* and is proportional to both n and n_t. We can put these ingredients together in order to write a rate equation of the form:

$$\frac{\partial n_t}{\partial t} = -G\,n_t + Rn(N - n_t) - Knn_t\,, \tag{1.20}$$

where the quantities G, R, and K are respectively called the coefficients of generation, capture, and impact ionization. We can immediately see that this rate equation is nonlinear in a qualitatively similar form as is found in the chemical reactions discussed in the previous section, cf. Eq. (1.6). It is also interesting to note that an additional feature not found in the chemical reaction literature is that the kinetic coefficients may have a strong dependence on electric field. As we shall see in Chapter 7, on trap-controlled space-charge instabilities, this feature plays a central role.

1.3 Structural Outline of the Book

We conclude this chapter by providing a road map of the presentation of material in this book. Chapters 2–4 are devoted to introducing key mathematical techniques that are especially useful for analyzing nonlinear wave phenomena in electronic transport systems. We begin in Chapter 2 by reviewing basic concepts and facts from nonlinear dynamics, including a summary of common bifurcations that are often encountered. Much of this material will be familiar to those who have previously studied nonlinear dynamics and, in this case, a fast reading is possible with the understanding that it can be referred to as necessary. In the second half of Chapter 2, we analyze bifurcations using a multiple scales approach known as the Chapman–Enskog method. This method has certain advantages in bifurcation analysis over the well-known normal form approach, especially for models of electronic transport. In Chapter 3, we introduce basic concepts of nonlinear waves in spatially continuous excitable media, illustrated using the FitzHugh–Nagumo and related models. Among the concepts presented are co-moving frame analysis, nonlinear wave speed determination methods, and stability analysis. In Chapter 4, we look at the application of these nonlinear wave methods to spatially discrete systems, especially periodic arrays where the new phenomena of wave pinning is expected to emerge.

Chapter 5 reviews the quantum mechanical underpinnings of the drift-diffusion transport models that are the focus of this book. After a discussion of fundamental quantum transport, we apply these methods to derive drift-diffusion currents for *strongly-coupled* semiconductor superlattices. Chapter 6 covers the theory of the Gunn effect in GaAs in which space charge instability is due to the peculiar nonlinear dependence of the drift velocity $v(E)$ on electric field. This chapter also begins with a self-contained review of the essential semiconductor physics underlying the Gunn effect. The concept of a greatly simplified asymptotic model for long samples is also introduced. In Chapter 7, we turn to the case where the instability is a result of field-dependent dynamics relative to trap states, also called trap-controlled instabilities. The treatment is largely parallel to that of the Gunn effect, though there are some striking differences between these two phenomena. In Chapter 8, we turn to the nonlinear dynamics of weakly-coupled semiconductor superlattices which are found moving as well as static (equivalently, pinned) electric field domains. It is

possible to understand many observed phenomena by applying singular perturbation methods to the limit $N_{SL} \to \infty$, where N_{SL} is the number of periods, or sequential layers of quantum wells, in the superlattice. Finally, in Chapter 9, we conclude with a brief and admittedly biased survey of some other systems in which the methods and tools developed here also provide useful insight.

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