An ecumenical nonlinear von Neumann equation: fluctuations, dissipation, and bifurcations

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An evolution equation is presented to describe the transport of a quantum mechanical quasiparticle such as an electron, or electronic or vibrational excitation, interacting strongly with lattice vibrations. A generalization of the discrete nonlinear Schrödinger equation to incorporate dissipation and fluctuation effects arising from interactions with a thermal reservoir, the equation predicts a multitude of interesting phenomena including bifurcations.

1. Introduction

Alwyn Scott has initiated, performed, stimulated, and guided, an amazing amount of current research in nonlinear physics. The community of nonlinear scientists owes much to him. It is a pleasure and an honour to be asked to make this contribution to the Festschrift on the occasion of his sixtieth birthday. The range of Alwyn's work in nonlinear science is vast. It spans a variety of systems and approaches, and deals with practical matters such as the problem of launching solitons and the spectra of acetanilide, as well as formal matters such as the dynamics of nonlinear systems and the generalization of nonlinearities [1–4].

The subject of the present article is the *ecumenical* nonlinear von Neumann equation

$$i\hbar \frac{d\rho_{mn}}{dt} = [V, \rho]_{mn} - \chi(\rho_{mm} - \rho_{nn})\rho_{mn}$$
$$- i\frac{\chi}{\Gamma}\rho_{mn}([V, \rho]_{mm} - [V, \rho]_{nn})$$
$$- i\alpha(1 - \delta_{mn})(\rho_{mn} - \rho_{mn}^{eq}). \tag{1}$$

Before describing the *what*, *whence*, and *whither* of this equation, it is relevant to comment on the

relation of the equation to Alwyn Scott. There exists a nonlinear transport equation which goes under the name of the discrete nonlinear Schrödinger equation (DNLSE), whose study has occupied many investigators, including the present author [5–8], for several years. Equation (1) is the augmented form taken on by the DNSLE, when the latter is opened to heat reservoirs and prepared for stochastic activities through the introduction of dissipation and fluctuation. The DNLSE, on the other hand, is identical in form to the so-called discrete self-trapping equation (DSTE), introduced earlier, and studied extensively, by Alwyn Scott and his collaborators.

While identical in form, and therefore in the relevance of a number of results such as concerning stationary states, the DSTE and the DNLSE differ significantly in physical meaning. This is evident from the role played by quantum mechanics in the two equations. The complex nature of the amplitudes in the DNLSE are a requirement of quantum mechanics and the study of the interplay of phases and nonlinearity is an undertaking of direct physical import. The complex nature of the amplitudes in the DSTE, on the other hand, is a convenience of the type familiar in electromagnetism where fields, which are actually real, are described by complex

quantities for computational ease. There is, thus, work on the "quantization" of the DSTE, which appears to have no counterpart at all in the context of the DNLSE. Also, the two equations differ in physical origin. We begin with a brief motivational discussion of the microscopic origin of the DNLSE in the next section. After a quick review of earlier work on the DNLSE in the following section, we introduce noninfinite relaxation and thermal fluctuations, and arrive at the ecumenical equation (1), which has been so termed because it is capable of resolving the competition and conflicts of nonlinearity and damping, or of fluctuation and dissipation, since it unifies the description of *all* these effects in one fell swoop. The fascinating consequences of the augmented equation will occupy us in the rest of the article. The subject under investigation is the transport of a low or intermediate mobility quasiparticle under strong interactions with vibrations. Examples are an electron in a narrow-band material, a vibrational or electronic excitation in a polymer, and a light interstitial such as a proton or muon in a metal. The notation in (1) is standard: ρ represents the density matrix of the quasiparticle, the matrix elements are taken in the representation of some localized states such as a Wannier set, and the four terms on the right side arise from intersite transfer, nonlinearity stemming from interactions with vibrations, finiteness of vibrational relaxation, and thermal fluctuations, respectively.

2. Physical motivation of the DNLSE

Consider a moving quasiparticle described by the ket $|\Psi(t)\rangle$ whose time evolution is governed by the Hamiltonian H through $i\hbar(d|\Psi(t)\rangle)/dt = H|\Psi(t)\rangle$, i.e., the standard Schrödinger equation. On multiplying the equation by a Wannier-like localized bra $\langle m|$, one obtains

$$i\hbar \frac{dc_m}{dt} = \sum_n V_{mn}c_n + E_m c_m , \qquad (2)$$

for the amplitudes c_m where the E's and the V's are, respectively, the diagonal and off-diagonal matrix elements of the Hamiltonian in the localized basis. If interactions with vibrations are present, the V's and E's are dependent on the vibrational coordinates x. For simplicity, let us take V_m to be independent of x, and E_m to depend linearly only on the internal coordinate x_m at site m. In the absence of interactions, x_m might have evolved sinusoidally with frequency ω and equilibrium position 0. It might naturally obey, in the presence of interactions,

$$\frac{d^2 x_m}{dt^2} + \omega^2 x_m = -\text{const.} \times |c_m|^2 , \qquad (3)$$

where the equilibrium position of the oscillator is changed by an amount proportional to the probability that site m is occupied by the quasiparticle. In the presence of a time scale disparity, if the vibrations are slaved by the quasiparticle probabilities, the time derivatives in (3) may be put equal to zero. The vibrational coordinate is then proportional to the quasiparticle occupation probability, and we obtain the DNLSE

$$i\hbar \frac{dc_m}{dt} = \sum_n V_{mn}c_n - \chi|c_m|^2 c_m . \qquad (4)$$

The above description of the origin of the DNLSE is meant to convey only its essential physical content. While we do not wish to discuss here the many subtleties which the microscopic derivation of the DNLSE entails [9,10], we now give a brief description of how the DNLSE can be obtained through a *semiclassical approximation* from the Hamiltonian evolution of the standard model of a quasiparticle interacting strongly with vibrations, viz.,

$$H = \sum_m \varepsilon_m a_m^\dagger a_m + \sum_{m,n} V_{m,n} a_m^\dagger a_n$$
$$+ \sum_q \hbar\omega_q (b_q^\dagger b_q + \tfrac{1}{2})$$
$$+ N^{-1/2} \sum_q \hbar\omega_q g_q$$
$$\times \exp(i q \cdot R_m) (b_q + b_{-q}^\dagger) a_m^\dagger a_m . \qquad (5)$$

Equation (5) uses standard notation which we will not detail here, except for stating that a and b refer, respectively, to the quasiparticle and the vibrations with which it interacts strongly. With

$$\hat{p} = a_1^\dagger a_1 - a_2^\dagger a_2 ,\tag{6a}$$

$$\hat{q} = -\mathrm{i}(a_1^\dagger a_2 - a_2^\dagger a_1) ,\tag{6b}$$

$$\hat{r} = a_1^\dagger a_2 + a_2^\dagger a_1 ,\tag{6c}$$

$$\hat{y} = -(b^\dagger + b)/2g ,\tag{6d}$$

the Hamiltonian (5) can be written, for a simple two-site symmetric system (a dimer) interacting with a single vibrational coordinate, as

$$H = V\hat{r} + g\omega\hat{p}(b^\dagger + b) + \omega(b^\dagger b + \tfrac{1}{2}) .\tag{7}$$

Here V denotes the interaction matrix element for the quasiparticle transfer between the two sites of the dimer, g measures the coupling strength with the vibration of frequency ω, and we have put the (identical) site energy of the two sites equal to zero: Henceforth we put $\hbar = 1$. Equation (7) then results in the following evolution for the quantities defined in (6):

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = 2V\hat{q} ,\tag{8a}$$

$$\frac{\mathrm{d}\hat{q}}{\mathrm{d}t} = -2V\hat{p} - \chi\hat{r}\hat{y} ,\tag{8b}$$

$$\frac{\mathrm{d}\hat{r}}{\mathrm{d}t} = \chi\hat{q}\hat{y} ,\tag{8c}$$

$$\frac{\mathrm{d}^2\hat{y}}{\mathrm{d}t^2} = -\omega^2(\hat{y} - \hat{p}) .\tag{8d}$$

Let us now take the expectation values of the operators in an initial state ψ, and denote these values by removing the circumflexes, i.e., $\zeta = \langle\psi|\hat{\zeta}|\psi\rangle$. *The single assumption that $\hat{y}$ is classical* converts the exact dynamics into the DNLSE, as it is trivial to show [6–8] that eqs. (8) rewritten without the circumflexes represent the DNLSE for the two-site system, the p, q and r being nothing other than the standard Feynman den-

sity matrix element combinations of the two-site system (dimer):

$$p = \rho_{11} - \rho_{22} , \quad q = \mathrm{i}(\rho_{12} - \rho_{21}) ,$$

$$r = \rho_{12} + \rho_{21} .\tag{9}$$

While simple, the foregoing demonstration makes transparent what crucial assumption is responsible for the passage from microscopics to evolution equations such as the DNLSE. It is clearly the assumption that the vibrations may be considered classical. This fact, while well known to many, has often gone unappreciated. This has led to numerous incorrect, although wishful, assertions on the one hand and meaningless queries on the other.

3. Nonlinear capture and trimer, N-mer evolution

Before proceeding with the process of the augmentation of the DNLSE into the ecumenical form (1), it is of interest to recall the large number of interesting and useful results which have emerged from the DNLSE in a variety of situations. Space limitations force us to do no more than list the primary contexts of some of that work, along with some slightly greater detail on two specific areas, viz. nonlinear trapping [11,12] and exact analysis of some spatially extended systems [13,14]. For further description, the reader may refer to several more detailed reviews [6–8].

The following is a list of some early work done on the DNLSE, i.e., from the infinite relaxation, zero temperature limit of (1):

(1) Exact solutions for the dynamics of the two-state system for arbitrary initial conditions and the elucidation of polaronic motion and self-trapping on the basis of those solutions [5].

(2) Application to fluorescence depolarization, wherein the moving quasiparticle is an electronic excitation and the observable is the

intensity of light emitted with different polarizations [6,15].

(3) Application to neutron scattering of hydrogen trapped around impurities such as oxygen in metals such as niobium, where the moving quasiparticle is the proton [16].

(4) Application to muon spin relaxation in antiferromagnetic solids such as bcc iron wherein the quasiparticle is a muon moving within a solid, and the observable is spin polarization [7,17].

(5) Generalization of the DNLSE to incorporate anharmonic potentials and nonlinear restoring forces, resulting in nonlinearities other than bilinear, and the appearance, and counterintuitive disappearance, of multiple stationary states [6,18].

(6) Calculation of memories in nonlinear generalized master equations, and the development of a perturbative scheme which is exact in the nonlinearity but perturbative in the intersite transfer [19].

(7) Studies of the interplay of nonlinearity and disorder on the basis of ensembles with various distributions of the nonlinearity parameter [6,7].

(8) Theory of nonlinear trapping of excitation directed at fluorescence quenching in molecular aggregates [11,12].

(9) Analytic solutions for a restricted class of initial conditions in some spatially extended systems such as trimers and symmetric N-mers [13,14].

We refer briefly to the last two of these below.

3.1. Nonlinear trapping

Quasiparticle trapping is an important phenomenon, and is of particular interest in areas of investigation such as photosynthesis, in which the harvesting of energy necessary for the operation of the reaction centers is followed by the process of the transfer of the harvested energy to the reaction center. The excitation carrying

energy, but no matter, is the quasiparticle, and the reaction center is the trap [20,21]. Let us assume that an excitation moves on a chain via nearest neighbour interactions V, and trapped by a site which has the nonlinear behavior arising from strong interactions with vibrations leading to the nonlinearity described by the cubic term in the DNLSE. Of the several possible models of capture, consider two: one in which one of the sites in the chain is itself the trap site and possesses the cubic nonlinearity, and another in which the excitation moves in a region of space called the antenna and communicates with a trap which is external to the antenna. In a simple example of the latter situation, the N antenna sites all communicate equally with the external trap through a matrix element W, while transferring excitation among themselves through nearest neighbour elements V. The first model is represented by

$$i \frac{dc_m}{dt} = V(c_{m+1} + c_{m-1}) - \delta_{m,0} \chi |c_0|^2 c_0 , \tag{10}$$

in obvious notation, while the second is represented by

$$i \frac{dc_m}{dt} = V(c_{m+1} + c_{m-1}) + Wc_\theta , \tag{11a}$$

$$i \frac{dc_\theta}{dt} = W \sum_m c_m - \chi |c_\theta|^2 c_\theta . \tag{11b}$$

Numerical calculations by Dunlap, Kenkre and Reineker [11] on the first model have shown that a transition appears to occur as the nonlinearity parameter χ crosses the value $(3.2)V$. The second model has been solved analytically by Kenkre and Kus' [12] who have shown that the probability of the trap site, which we will call P, obeys

$$\frac{d^2P}{d\tau^2} = \frac{1}{2}(I_1 - \eta I_2) - (\xi I_2 + \eta^2 + 1)P$$

$$- 3\xi \eta P^2 - 2\xi^2 P^3 , \tag{12}$$

where, with the notation that w is defined as $\sqrt{N} W$, the scaled time τ and the parameters ξ

and η are $\tau = 2wt$, $\xi = \chi/4w$, and $\eta = V/w$, the Γ's being constants of the motion. Clearly, ξ measures the amount of nonlinearity relative to the (scaled) interaction matrix element for transfer of excitation between the antenna and the trap while η measures the motion of the excitation within the antenna relative to the extent of its transfer from the antenna to the trap. Equation (12) can be solved in terms of Weierstrassian elliptic functions. A completely general solution to the problem has been obtained for arbitrary initial conditions, and a number of physical features have been extracted [12]. The analysis has also been generalized to finite relaxation and finite temperature situations.

3.2. Spatially extended systems: analytic results

The methods of analysis used in the early work [5] to obtain exact solutions in two-site systems were generalized by Andersen and Kenkre to some larger systems including trimers and a class of extended systems termed N-mers [13,14]. They obtained the explicit time dependence for the trimer for a class of special initial conditions, discussed a transition at $\chi = -6V$ as well as the effect of the sign of the nonlinearity, and showed the connection of their results to the trimer stationary states obtained earlier by Eilbeck et al. [3]. They generalized the work to N-mers, also obtaining explicit analytical solutions. The systems considered were site-degenerate with $V_{mn} = V$ between any two sites, the initial excitation being localized on a single site, or more generally, distributed equally among all sites of one of two groups, one of m_A sites and the other of $m_B = N - m_A$ sites. The calculational trick of Andersen and Kenkre [13,14] consists of the generalization of (9) to define new quantities p, q, and r, which allow one to convert the trimer or N-mer problem as described by

$$\frac{dc_m}{dt} = -iV\left(-c_m + \sum_n c_n\right) + i\chi|c_m|^2 c_m , \qquad (13)$$

into a completely tractable non-degenerate dimer problem [22] involving the solution of

$$\frac{d^2 p}{dt^2} = -2\gamma_0 - 6\gamma_1 p - 6\gamma_2 p^2 - 2\gamma_3 p^3 . \qquad (14)$$

Some of this work is reappearing in the literature and is being applied to experimental situations.

4. Finite relaxation and thermal fluctuations

How do we augment the DNLSE (4) to treat situations not involving time scale disparities between the quasiparticle and the vibrations, to eliminate unrealistic assumptions such as that of infinite vibrational relaxation, and to include unavoidable, and important, interactions with reservoirs which give rise to temperature effects and fluctuations? This is the question that we now address. Equation (4) is the result of a time disparity assumption made on (2) and (3). We now retain (2), and replace (3) by

$$\frac{d^2 x_m}{dt^2} + \gamma \frac{dx_m}{dt} + \omega^2 x_m = -\text{const.} \times |c_m|^2 + R_m(t) , \qquad (15)$$

and explore the consequences of dissipation introduced by the rate γ, and of fluctuation caused by the random force term $R_m(t)$. For simplicity, we have used the restriction that the reservoir interaction occurs only with the vibrational system. Two limits of (15) are particularly interesting: zero damping, and extremely large damping. Some exact solutions can be found for the former case [23] for the dimer. The probability difference $p(t)$ shows cn or dn behavior as in the adiabatic solutions [5] and undergoes a characteristic new transition into a region where it equals the sum of a part which is proportional to the appropriate elliptic function (cn or dn), and a part which is proportional to the cube of the elliptic function. Here, we will focus on the opposite limit of extremely large damping.

If the damping is large enough to justify the

neglect of the second derivative of the oscillator displacements, more formally, if $\omega \to \infty$, $\gamma \to \infty$, $\omega^2/\gamma = \Gamma$, the evolution of the oscillator displacements towards their equilibrium positions now possesses a single characteristic "vibrational relaxation" rate Γ. Restricting the analysis to the two-site system in the interest of full tractability, we obtain from (2) and the large damping limit of (15),

$$\frac{dp}{dt} = 2Vq , \quad \frac{dq}{dt} = -2Vp - \chi yr , \quad \frac{dr}{dt} = \chi yq ,$$
$$\tag{16a}$$

$$\frac{dy}{dt} = -\Gamma(y - p) + F(t) , \quad F(t) = 2\Gamma(kT/\omega^2)\delta(t) ,$$
$$\tag{16b}$$

where k is the Boltzmann constant.

Equations (16) constitute a Langevin set. Standard techniques allow the derivation of an exact Fokker–Planck equation for the distribution function in p, q, r, y space and of an approximate but useful Fokker–Planck equation for the distribution function $\sigma(p, q, r; t)$ in p, q, r space alone. The latter is obtained [24] through the application of projection techniques which eliminate the vibrational variable y, and is valid in the high damping limit. The Fokker–Planck equation can be solved exactly for its stationary state distribution function, and the formalism can be used in two separate ways: (i) to perform a Kramer's first passage time analysis aimed at an investigation of the stability (against thermal fluctuations) of the nonlinear structures inherent in the DNLSE, and (ii) to carry out a contraction analysis [25] from the Fokker–Planck equation in order to arrive at a closed equation such as (1) for the quasiparticle variables. We refer the reader elsewhere [24] for (i), and concentrate on the results of (ii) here. The contraction analysis has, as its consequence,

$$\frac{dp}{dt} = 2Vq ,$$
$$\tag{17a}$$

$$\frac{dq}{dt} = -2Vp - \chi pr + \frac{2V\chi}{\Gamma} qr - \alpha q ,$$
$$\tag{17b}$$

$$\frac{dr}{dt} = \chi pq - \frac{2V\chi}{\Gamma} q^2 - \alpha(r - r_{eq}) .$$
$$\tag{17c}$$

Here, r_{eq} is the thermal equilibrium value of r, and α is a rate which attempts to drive the system to the thermal state. A high temperature expression [25] for this rate is $\alpha = (2\chi/\Gamma)kT$.

The set of equations (17) have been arrived at by extending the DNLSE to nonadiabatic, finite temperature situations through a blend of analytic arguments and physical assumptions. The system they describe reduces to the trivial linear dimer if $\chi = 0 = \alpha$, to the high-temperature damed linear dimer if χ vanishes but α does not, to the nonlinear adiabatic dimer if χ is finite but Γ is infinite and α vanishes, to a relatively crude extension [26] of the nonlinear dimer to dissipative situations if χ is finite but Γ is infinite and α vanishes, and to the nonlinear nonadiabatic dimer if χ and Γ are finite and α vanishes. The latter case displays a rich multitude of phenomena including a fascinating interplay of quantum phases and nonlinearity, for which we refer the reader to refs. [27]. Evolution showing a complete combination of the elliptic function evolution of the adiabatic dimer for short times, followed by a self-trapping swing into the localized stationary states of the dimer for longer times, which is itself followed by a delocalization and symmetrical spreading over the two sites characteristic of thermal fluctuations, has been exhibited and commented on in ref. [25] for the high-temperature case when r_{eq}, which can generally be taken to equal $\tanh(V/kT)$, vanishes. Exciting new behavior, which occurs when r_{eq} does *not* vanish, will now be mentioned here briefly.

For vanishing α, the probability difference p oscillates and then tends to the stationary value which is 0 if the nonlinearity parameter is small enough and finite (corresponding to a localized state) if it is large enough. As α increases, the detrapping effect is seen: p tends to 0 at larger times even for large nonlinearities. As α increases further, a surprising burst of p occurs for

a short time, and the burst recurs after a time period. The bursts become more frequent with further increase of α and behavior that *appears* chaotic occurs. Phase space plots in the p-q plane show that a limit cycle has been reached at this point, as p (as well as q) oscillates steadily between two finite values (see (iv) and (v) in fig. 1). A further increase in α destroys the limit cycle, and stable dissipative behavior is recovered (case (vi)): p, q tend to vanishing values while r tends to r_{eq}. Stability analysis carried out

by Kenkre and Kuś [26] shows that the destruction of limit cycles occurs for $\alpha > r_{eq}\chi/\Gamma$, i.e., for temperatures exceeding that at which V/kT becomes smaller than its hyperbolic cotangent if χ and Γ are assumed to be independent of temperature.

This bifurcation behavior is reflected in exciting predicted features of several observable quantities [26]. An example is the degree of fluorescence polarization in poly-L-proline oligomers of variable length, which is given [6] by a
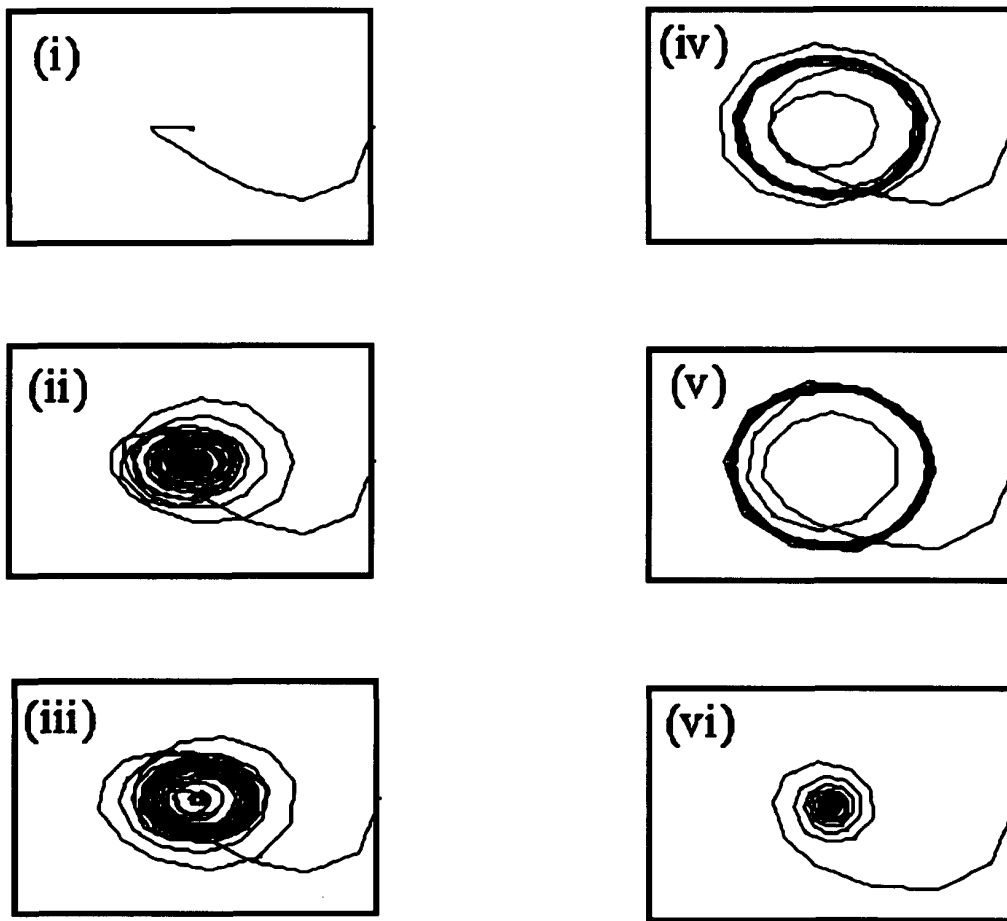

Fig. 1. p-q phase space plots from (17), the dimer form of (1), showing bifurcaton behavior. Each frame extends from -1 to 1 on the horizontal p and the vertical q axis, and the initial condition is of one-site occupation, i.e., $p = 1$, $q = 0$. The nonlinearity $\chi/2V$ is larger than 1: localized states exist. The values of $\alpha/2V$ are (i) 0.002, (ii) 0.00968, (iii) 0.04685, (iv) 0.22676, and (vi) 1.09752. In (i), one sees clear evolution to the self-trapped stationary state ($p < 0$) followed by symmetrization ($p = 0$) as a result of thermal fluctuation. Limit cycles are destroyed in (vi).

linear superposition of p and r, the coefficients of the superposition being subject to experimental control.

5. Concluding remarks

The derivation of (1) has proceeded through a combination of exact analysis and physical arguments. The semiclassical approximation which yields the DNLSE, the reservoir interaction, also introduced classically, which results in the Fokker–Planck equation, the high damping limit, the contraction analysis from the Fokker–Planck equation, and the generalization from the dimer back to the extended system necessary to pass from (17) to (1), are the primary ingredients of that combination. We have seen the rich behavior that emerges from (1). It encompasses simple linear evolution, reflects the characteristic features of nonlinear dynamics, describes the settling of the system into stationary states as a result of dissipation and finite relaxation, and predicts fascinating bifurcations. What is required in future investigations, in the opinion of the present author, is not only a better understanding of the range of validity and applicability of this and similar transport instruments, but also (and especially) work on the *design of specific experiments* on the basis of the kind of theoretical predictions that have been described in the present article. The depolarization of fluorescence, the scattering of probe particles such as neutrons by light interstitials, the quenching of fluorescence via trapping, and the evolution of transient gratings are particular candidates for the experimental probe. It is hoped that the development of theoretical analysis and the design of experiments will occur in close collaboration in the near future.

Acknowledgements

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