

Generalized master equations from the nonlinear Schrödinger equation and propagation in an infinite chain

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Generalized master equations with nonlinear memory functions describing quasiparticle transport on lattices are derived explicitly from the discrete nonlinear Schrödinger equation through the application of diagonalizing projection operators. Exact results are presented for dimers, and an approximation scheme is developed for extended systems such as an infinite chain, which treats the nonlinearity exactly and the intersite transfer perturbatively. An apparent connection to the Toda lattice is pointed out. The exact results presented for the dimer include an explicit evaluation of the initial (driving) term in the generalized master equation.

I. INTRODUCTION

One encounters the discrete nonlinear Schrödinger equation in the context of numerous phenomena in various fields of physics.¹⁻¹⁰ The equation may be written, in its simplest form, as

$$\frac{dc_m(t)}{dt} = -iV(c_{m+1} + c_{m-1}) + i\chi|c_m|^2c_m. \quad (1.1)$$

Here c_m is the amplitude for the system to be in the state $|m\rangle$ which is localized at the m th site in the one-dimensional crystal considered here, V is the interstate matrix element [assumed "nearest neighbor" in (1.1)] describing the evolution among the states $|m\rangle$, and χ is the nonlinearity parameter of special importance to the present investigation. The matrix element V is proportional to the bandwidth of the bare electron or exciton, and the nonlinearity χ is nothing other than the energy lowering due to polaronic effects, often written as a sum of the products of the vibrational energies of the participating modes and the square of their coupling constants with the electron or exciton.

Solutions to Eq. (1.1) are not known in general. Some of the solutions are known in the continuum limit⁹ and the entire evolution is known analytically⁵⁻⁸ for a two-site system—the dimer—but one has had to rely on numerical methods¹⁰ to investigate excitation transport which obeys (1.1) in an extended system. In the present paper we shall show that, starting from (1.1), it is possible to derive a generalized master equation (GME) governing the evolution of the probabilities of site occupation, that the memory functions appearing in the equation are explicitly nonlinear in the probabilities, that an approximation scheme can be developed on the basis of the GME which can address nonlinearity to all orders but intersite transfer to small orders, and that a curious relation appears to exist between the approximated GME and the Toda lattice equation.¹¹ As a preliminary to the derivation of the GME we present the Liouville–Von Neumann equation obeyed by the density matrix ρ_{mn} . Equation (1.1) and its complex conjugate can be combined to give⁵

$$\begin{aligned} \frac{d\rho_{mn}}{dt} = & -iV(\rho_{m+1n} + \rho_{m-1n} - \rho_{mn+1} - \rho_{mn-1}) \\ & + i\chi(\rho_{mm} - \rho_{nn})\rho_{mn} \end{aligned} \quad (1.2)$$

provided χ is assumed real. As we have pointed out elsewhere,^{5,6} a linear chain with statically varying site energies (as in a disordered chain) would obey (1.2) with the replacement of the second term $i\chi(\rho_{mm} - \rho_{nn})\rho_{mn}$ by the energy mismatch term $-i(E_m - E_n)\rho_{mn}$, where E_m is the site energy at m . The energy lowering $-\chi\rho_{mm}$ which equals the product of χ and the probability of occupation of site m is clear in (1.2).

II. THE NONLINEAR GENERALIZED MASTER EQUATION

Unlike the standard Liouville–Von Neumann equation which is a linear equation, (1.2) is nonlinear. It would, therefore, appear that linear techniques such as those involving the diagonalizing projection operators of Zwanzig¹² would not be useful in its analysis. We shall show, however, that, this is not true: despite its nonlinearity, (1.2) can indeed be approached profitably with the projection technique. We rewrite (1.2) in the symbolic form

$$\frac{d\rho}{dt} = -iL_V\rho + iL_\chi\rho = -iL\rho \quad (2.1)$$

where the "Liouville" operators L_V and L_χ are defined through

$$L_V O = [V, O], \quad (2.2)$$

$$(L_\chi O)_{mn} = \chi(\rho_{mm} - \rho_{nn})O_{mn} \quad (2.3)$$

for any operator O . If, in the manner of Zwanzig, we apply diagonalizing projection operators P and $1 - P$ to (2.1) via the definition

$$(PO)_{mn} = O_{mn}\delta_{mn} \quad (2.4)$$

we obtain¹² the two equations

$$\frac{d\rho'}{dt} = -iPL\rho' - iPL\rho'' , \quad (2.5)$$

$$\frac{d\rho''}{dt} = -i(1-P)L\rho'' - i(1-P)L\rho' . \quad (2.6)$$

The definition of L_χ that we have introduced through (2.3) has been constructed specifically to allow the application of linear projection operators to the nonlinear density matrix equation (1.2). A natural alternative to (2.3) could have been

$$(L_\chi O)_{mn} = \chi(O_{mm} - O_{nn})O_{mn} . \quad (2.7)$$

Such a choice would make both (2.5) and (2.6) nonlinear. The definition we have introduced, however, has the consequence that, while (2.5) is a nonlinear equation for ρ' , the diagonal part of the density matrix, (2.6), is a linear equation for ρ'' , the off-diagonal part. This is so because (2.3) shows that the action of L_χ on the off-diagonal part ρ'' involves multiplication by elements of the diagonal part of the density matrix. We can thus solve (2.6) and substitute in (2.5) through standard methods of linear differential equations exactly as in the completely linear cases of Zwanzig and others.¹²⁻¹⁵ The result is the well-known equation

$$\frac{d\rho'}{dt} = -iPL\rho' - PL \int_0^t ds \left[\exp \left[-i \int_s^t dz (1-P)L(z) \right] \right] \times (1-P)L(s)\rho'(s) \quad (2.8)$$

valid for the initial random-phase condition that ρ is initially diagonal. If such a condition does not apply, (2.8) contains an additional driving term.^{12,16} We shall not be concerned with non-random-phase initial conditions in the main body of the present paper. In the Appendix we shall evaluate the initial term and discuss its consequences for the two-site system. Standard arguments show that the first term on the right-hand side of (2.8) vanishes identically, and (2.8) can be written in the GME form:

$$\frac{dP_m(t)}{dt} = \int_0^t ds \sum_n [\mathcal{W}_{mn}(t,s)P_n(s) - \mathcal{W}_{nm}(t,s)P_m(s)] , \quad (2.9)$$

where the nonlinear memory functions $\mathcal{W}_{mn}(t,s)$ are obtained from the elements of the tetradic

$$PL \int_0^t ds \left[\exp \left[-i \int_s^t dz (1-P)L(z) \right] \right] (1-P)L(s)\rho'(s) .$$

III. EXACT REDUCTION FOR THE DIMER AND RECOVERY OF KNOWN RESULTS

The disentangling of the projection operators in (2.8) can be done without approximation when the system under consideration is a dimer. Equation (2.3) shows that, when acting on the diagonal part ρ' of the density matrix, L_χ produces a vanishing result. This has the consequence that

$$\langle 1 | (1-P)L(s)\rho'(s) | 2 \rangle = -V[\rho_{11}(s) - \rho_{22}(s)] . \quad (3.1)$$

Arbitrary powers n of the operator $(1-P)L(z)$ acting on the right-hand side of (3.1) yield the following result:

$$\begin{aligned} \langle 1 | [(1-P)L(z)]^n (1-P)L(s)\rho'(s) | 2 \rangle \\ = (-1)^{n+1} \chi^n V [\rho_{11}(s) - \rho_{22}(s)] [\rho_{11}(z) - \rho_{22}(z)]^n . \end{aligned} \quad (3.2)$$

The series produced by the action of $\exp[-i \int_s^t dz (1-P)L(z)]$ on the right-hand side of (3.1) can thus be summed explicitly to yield a sum of two terms which are respectively proportional to the cosine and the sine of the expression $\int_s^t dz \chi [\rho_{11}(z) - \rho_{22}(z)]$. The sine term vanishes as a consequence of the action of $PL(t)$ on this expression. The final result is the following set of coupled equations of motion for the probabilities $\rho_{11}(t)$ and $\rho_{22}(t)$ which describe the site occupation at the sites 1 and 2 of the dimer:

$$\begin{aligned} \frac{d\rho_{11}(t)}{dt} = 2V^2 \int_0^t ds [\rho_{22}(s) - \rho_{11}(s)] \\ \times \cos \left[\int_s^t dz \chi [\rho_{22}(z) - \rho_{11}(z)] \right] , \end{aligned} \quad (3.3)$$

$$\begin{aligned} \frac{d\rho_{22}(t)}{dt} = 2V^2 \int_0^t ds [\rho_{11}(s) - \rho_{22}(s)] \\ \times \cos \left[\int_s^t dz \chi [\rho_{22}(z) - \rho_{11}(z)] \right] . \end{aligned} \quad (3.4)$$

Equations (3.3) and (3.4) constitute the exact nonlinear generalized master equation for the dimer. They are rather different in appearance from those describing the exact evolution of the dimer probabilities derived by Kenkre and Campbell.⁵ To show their equivalence to the result of Ref. 5, we subtract (3.4) from (3.3) to obtain the closed equation of evolution for the difference p of the probabilities $P_1 - P_2$:

$$\frac{dp(t)}{dt} + 4V^2 \int_0^t ds p(s) \cos \left[\chi \int_s^t dz p(z) \right] = 0 . \quad (3.5)$$

We now define a new quantity $\xi(t)$ through

$$\xi(t) = \int_0^t ds p(s) . \quad (3.6)$$

Equation (3.5) is then reduced to a second-order differential equation for $\xi(t)$:

$$\frac{d^2 \xi(t)}{dt^2} + (4V^2/\chi) \sin[\chi \xi(t)] = 0 . \quad (3.7)$$

Equation (3.7) is the well-known pendulum equation, has appeared recently in the work of Cruzeiro-Hansson *et al.*,¹⁷ and can be solved immediately to yield

$$\xi(t) = (2/\chi) \sin^{-1}[\text{sn}(\chi t/2 | 4V/\chi)] . \quad (3.8)$$

Finally, the differentiation of (3.8) with respect to t gives

$$p(t) = d\xi/dt = \text{cn}(2Vt | \chi/4V) \quad (3.9)$$

if $p(0) = 1$ and $(dp/dt)_0 = 0$. In Eqs. (3.8) and (3.9) the sn and cn are the Jacobian sine and cosine elliptic functions and the factor following $|$ in their expressions is their elliptic parameter. Equation (3.9) is the exact dimer result

derived in Ref. 5. It is also possible, if desired, to show that (3.3) leads directly to the evolution equation

$$\frac{d^2 p}{dt^2} = Ap - Bp^3, \quad (3.10)$$

where the constants A and B are given by initial conditions (as in Refs. 5–8).

IV. APPROXIMATE MEMORY FUNCTIONS FOR THE CHAIN

While the exact evaluation of the memory functions in (2.9) is possible only for the dimer, an approximation scheme can be developed for the chain. Since our interest is primarily in the nonlinearity, it is important that we not treat it perturbatively. On the other hand, the site-to-site transfer may be considered to be weak enough to be analyzed via an approximation. We thus apply to (2.8) the standard weak-coupling approximation wherein L_v is taken to have a small effect compared to the effect of the nonlinearity. We first note that the tetradic shown at the end of Sec. II can be written as

$$PL_v \int_0^t ds \left[\exp \left[-i \int_s^t dz (1-P)L(z) \right] \right] L_v \rho'(s),$$

where the first and the last L have been written *without approximation* as L_v . This is simply a consequence of the nature of P and of L_χ . We now invoke the weak-coupling approximation: the action of L_v is taken to be small (in the sense of a perturbation) with respect to that of L_χ . The lowest nonvanishing term in an expansion of the tetradic in powers of L_v is then

$$PL_v \int_0^t ds \left[\exp \left[+i \int_s^t dz L_\chi(z) \right] \right] L_v \rho'(s).$$

In writing the above we have made use of the fact that L_χ acting on any operator produces an operator which is completely off diagonal in the representation of m, n , etc. The expansion of the exponential in powers of $+i \int_s^t dz L_\chi(z)$ and the use of the definition of L_χ gives

$$\begin{aligned} & \left[\exp \left[+i \int_s^t dz L_\chi(z) \right] O \right]_{mn} \\ &= \left[\exp \left[+i \int_s^t dz \chi [\rho_{mm}(z) - \rho_{nn}(z)] \right] \right] O_{mn}. \end{aligned} \quad (4.1)$$

It is straightforward to use (4.1) in (2.8) to obtain

$$\frac{dP_m(t)}{dt} = \int_0^t ds \sum_n [\mathcal{W}_{mn}(t,s)P_n(s) - \mathcal{W}_{nm}(t,s)P_m(s)], \quad (2.9)$$

the nonlinear memory functions being given by

$$\begin{aligned} \mathcal{W}_{mn}(t,s) &= 2V^2(\delta_{m,n+1} + \delta_{m,n-1}) \\ &\quad \times \cos \left[\chi \int_s^t dz [P_m(z) - P_n(z)] \right]. \end{aligned} \quad (4.2)$$

The properties of the projection and Liouville operators which allow the exact evaluation of the nonlinear memory functions for the dimer and the approximate evaluation for the extended system given above are simi-

lar to those used by one of the present authors in the exact evaluation¹⁸ of the memory functions from a stochastic Liouville equation. The latter is the same as (2.1) but with (2.3) replaced by

$$(L_\chi O)_{mn} = \alpha(1 - \delta_{m,n})O_{mn}. \quad (4.3)$$

In the series expansion of the tetradic mentioned above, $(1-P)L_\chi$ and $(1-P)L_v$ commute for the case of Ref. 18 but not in the present case. The primary difference is that successive powers of $(1-P)L_\chi$ introduce simply multiplicative powers of the c number α in the case of the stochastic Liouville equation treated in Ref. 18 but products of different quantities in the case of the nonlinear Liouville equation considered here. The result is that, in the present case, an exact solution is possible through the above methods for the two-state system but not for systems of arbitrary size.

Equation (4.2) along with (2.9) is the nonlinear generalized master equation in the weak-coupling approximation for the intersite transfer. The approximation inherent in (4.2) is of a weak-coupling nature in V and not in the nonlinearity χ . The latter is taken to infinite order and the former to the lowest nonvanishing order. The approximation is exact for the case of a two-site chain as we have demonstrated in Sec. III. For extended systems it inherits the features of its linear counterpart. It is well known^{15,19} that the weak-coupling memory functions in the linear case produce negative probabilities but yield the exact mean-square displacement or velocity autocorrelation function. Thus, while calculations of probabilities or related quantities with the weak-coupling approximation must be undertaken with care, it is well suited to the calculation of moments of probability, mean-square displacements, velocity correlation functions, diffusion constants, and effective transfer rates.

In Fig. 1 we compare the mean-square displacements

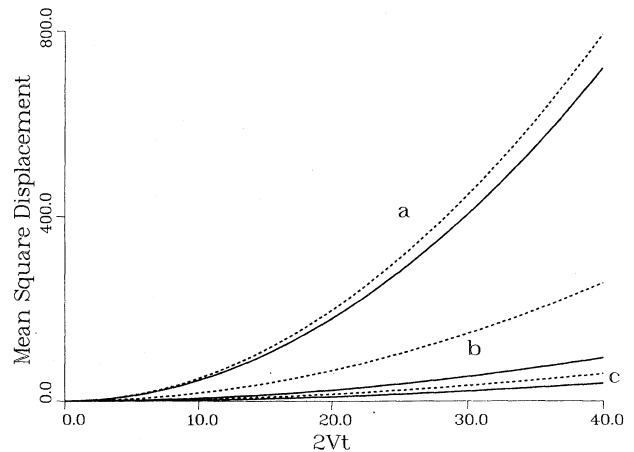


FIG. 1. The mean-square displacement (arbitrary units) plotted as a function of time in units of $1/2V$ for various values of the nonlinearity ratio $\chi/4V$: (a) 0.5, (b) 1.25, and (c) 2. The solid lines represent the exact evolution while the dashed lines are obtained from solutions of the weak-coupling nonlinear generalized master equation.

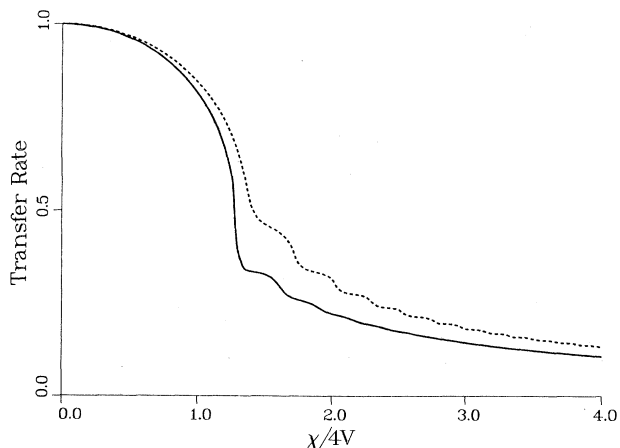


FIG. 2. The (normalized) transfer rate, defined as the reciprocal of the time taken for the mean-square displacement of an initially site-localized particle to attain the value a^2 , where a is the lattice constant, plotted as a function of the nonlinearity. The qualitative features of the exact solution (solid line) are reproduced by the solution of the weak-coupling generalized master equation (dashed line) and the change from “free” to “self-trapped” behavior (large to small values of the rate) is seen clearly.

as given by the GME (2.9) through our approximation (4.2) for the nonlinear memory functions to the exact result from (1.1). There are obtained numerically. We find that the qualitative behavior of the time dependence appears quite similar in the two cases and that the difference is large for values of the nonlinearity χ near the transition from free to self-trapped motion. In order to examine the transition more carefully, we define a transfer rate²⁰ as the reciprocal of the time taken for the mean-square displacement to change from the value 0 to a^2 , where a is the intersite distance (lattice constant) and plot the transfer rate (see Fig. 2) as a function of the nonlinearity. The transfer rate we have defined is a measure of how quickly the quasiparticle moves to its neighboring site from the site of initial localization. The comparison of the exact and the approximate results shows that the latter corresponds to motion which is faster than actual, that the difference of the two results is largest near the transition region, and, what is most important, that the qualitative features of the rate, including the transition, are preserved under the approximation.

V. CONCLUDING REMARKS

The contributions of this paper are an exact derivation of a nonlinear generalized master equation starting from the nonlinear Schrödinger equation, an exact evaluation of the nonlinear memory functions (and of the initial condition term for arbitrary initial conditions) in the case of the dimer, and an approximate evaluation of the memory functions in the case of an extended system such as chain or higher-dimensional crystal. These include Eqs. (2.9), (3.3), (3.4), and (4.2), and (5.5) and (5.6). We have shown that an application of the *linear* projection operators to the nonlinear Von Neumann equation is made feasible by a formal linearity of the Zwanzig projected equation for

the off-diagonal part of the density matrix. In our exact evaluation of the memory functions we have found that they have the standard form^{12,15}

$$\mathcal{W}_{mn}(t,s) = 2V^2 \cos \left[\int_s^t dz (E_m - E_n) \right], \quad (5.1)$$

the site energies E_m and E_n being, however, proportional to the probabilities themselves as a result of the nonlinearity of the evolution equation. Previous dimer work of Brown *et al.* has also resulted in nonlinear memory functions similar to ours.⁴

The approximation scheme that we have developed for the calculation of the memory functions in extended systems treats the nonlinearity exactly but the intersite transfer to small order. It is thus applicable to the description of transport of quasiparticles in “narrow-band” materials. The resulting equation has not yet allowed an analytic solution. But we have seen that it is capable of describing the primary qualitative features of the motion, in particular the self-trapping transition. It is hoped that analytic work will be facilitated by the weak-coupling memory function in future investigations.

Both the GME’s, the exact one for the dimer, and the approximate one for the extended systems, find particular use in the study of the interplay of randomness with nonlinearity. The nonlinearity parameter χ depends for its value on the magnitude of the interaction of the moving particles with the vibrations of the lattice and on the frequencies of the vibrations. These frequencies and the coupling constants could vary from site to site and be therefore regarded as random parameters. The nonlinearity parameter χ would thus itself be a random quantity, the situation being analogous to inhomogeneous broadening of spectral linewidths or dephasing of spins in nuclear magnetic resonance experiments. A detailed theory of the effects of the interplay of such randomness with nonlinearity, particularly in dimers, forms the content of a forthcoming publication.²¹ Here we would like to anticipate the results of that discussion and show that the introduction of randomness into the nonlinear GME can make the latter remarkably similar in appearance to the equation of evolution for the Toda lattice¹¹ in a nonlinear chain.

Assume that, in our system, randomness may be described by considering an ensemble of members, each with a specific value of χ , in such a way that the evolution is described by the average (over the ensemble) of the memory functions:

$$\mathcal{W}_{mn}^{\text{eff}}(t,s) = \int d\chi \rho(\chi) \mathcal{W}_{mn}(t,s,\chi) \quad (5.2)$$

where \mathcal{W}^{eff} is the effective memory function, $\rho(\chi)$ is the distribution function of the nonlinearity parameter χ , and $\mathcal{W}_{mn}(t,s,\chi)$ is given by (4.2). It is clear then that for a distribution function which is a Lorentzian of width α , the effective memory function \mathcal{W}^{eff} has an exponential dependence on the argument $\int_s^t dz [P_m(z) - P_n(z)]$. As an extension of the dimer definition (3.6) to the chain, we define the quantities

$$\xi_m(t) = \int_0^t dz P_m(z) \quad (5.3)$$

and obtain, at once, the generalization of the evolution equation (3.7) applicable to the chain:

$$\frac{d^2\xi_m}{dt^2} = (\pi V^2/\alpha) [\exp(-\alpha|\xi_m - \xi_{m-1}|) - \exp(-\alpha|\xi_{m+1} - \xi_m|)] . \quad (5.4)$$

Equation (5.4) is remarkably similar to the evolution equation for the Toda lattice, which is

$$\frac{d^2\xi_m}{dt^2} = \text{const} \times \{ \exp[-\alpha(\xi_m - \xi_{m-1})] - \exp[-\alpha(\xi_{m+1} - \xi_m)] \} , \quad (5.5)$$

the only difference between (5.4) and (5.5) being that the absolute values of the differences of ξ_m at neighboring sites appear in the former while their actual values appear in the latter.

Investigations are under way on exploring the significance of this connection as well as on developing approximate analytic solutions of the weak-coupling GME, extensions of the perturbation to higher orders in the intersite transfer, and exact evaluation of the memory functions for small systems larger than a dimer.

APPENDIX

The generalized master equation which we derived in Sec. III was obtained under the assumption of initial random phases. In this appendix we present the *complete* GME for arbitrary initial conditions in the case of the two-site system. The general form of the GME obtained through the application of diagonalizing projection operators as shown in Sec. II is

$$\frac{d\rho'}{dt} = -PL \int_0^t ds \left[\exp \left[-i \int_s^t dz (1-P)L(z) \right] \right] \times (1-P)L(s)\rho'(s) + I(t) . \quad (A1)$$

Equation (A1) is an *exact* consequence of (2.1). It differs from (2.8) through the presence of the driving term $I(t)$. The term vanishes under the initial random phase or localized condition [for which $(1-P)\rho(0)=0$, or more generally¹⁶ whenever $L(1-P)\rho(0)=0$], allowing the recovery of (2.8) from (A1). Generally, the initial term $I(t)$ is given by

$$I(t) = -iPL \left[\exp \left[-i \int ds (1-P)L(s) \right] \right] (1-P)\rho(0) . \quad (A2)$$

We expand the exponential in (A2) and notice that, for a dimer, $(1-P)L_V(1-P)$ acting on any operator produces

a vanishing result. This allows the replacement of L by L_χ in the exponential in (A2). On carrying out the action of the series on $(1-P)\rho(0)$ explicitly, we obtain the complete GME:

$$\frac{dP_1(t)}{dt} = \int_0^t ds [\mathcal{W}_{12}(t,s)P_2(s) - \mathcal{W}_{21}(t,s)P_1(s)] + I_1(t) , \quad (A3)$$

$$\frac{dP_2(t)}{dt} = \int_0^t ds [\mathcal{W}_{21}(t,s)P_1(s) - \mathcal{W}_{12}(t,s)P_2(s)] + I_2(t) . \quad (A4)$$

The memories $\mathcal{W}_{mn}(t,s)$ have been evaluated in Sec. II:

$$\begin{aligned} \mathcal{W}_{12}(t,s) &= \mathcal{W}_{21}(t,s) \\ &= 2V^2 \cos \left[\chi \int_s^t dz [P_1(z) - P_2(z)] \right] . \end{aligned} \quad (A5)$$

Introducing the notation

$$r = (\rho_{12} + \rho_{21}), \quad q = i(\rho_{12} - \rho_{21}) , \quad (A6)$$

recalling that $p = P_1 - P_2$, and using the evaluation detailed above, we find the driving terms given by

$$I_1(t) = -Vr_0 \sin \left[\chi \int_0^t dz p(z) \right] + q_0 \cos \left[\chi \int_0^t dz p(z) \right] , \quad (A7)$$

$$I_2(t) = +Vr_0 \sin \left[\chi \int_0^t dz p(z) \right] - q_0 \cos \left[\chi \int_0^t dz p(z) \right] . \quad (A8)$$

Equations (A3) and (A4), with the memories and the driving terms given by (A5)–(A8), constitute the exact and complete probability evolution in the quantum nonlinear dimer for arbitrary initial conditions.

The definition of the quantity $\xi(t)$ through

$$\xi(t) = \int_0^t ds p(s) = \int_0^t ds [P_1(s) - P_2(s)] \quad (3.6')$$

converts the full GME into a second-order differential equation for ξ :

$$\frac{d^2\xi}{dt^2} + M \sin(\chi\xi) - N \cos(\chi\xi) = 0 , \quad (A9)$$

$$M = (4V^2/\chi) + 2Vr_0, \quad N = 2Vq_0 . \quad (A10)$$

Equation (A9), which is the generalization of (3.7) valid for arbitrary initial conditions, can be solved explicitly for ξ and can also be used through ξ potentials for a direct study of the dimer transitions reported earlier.^{5,8} The details will be presented elsewhere.

¹A. C. Scott, F. Y. Chu, and D. W. McLaughlin, Proc. IEEE **61**, 1443 (1973).

²A. S. Davydov, J. Theor. Biol. **38**, 559 (1973); Usp. Fiz. Nauk. **138**, 603 (1982) [Sov. Phys.—Usp. **25**, 898 (1982)], and references therein.

³J. C. Eilbeck, P. S. Lomdahl, and A. C. Scott, Physica D **16**, 318 (1985).

⁴D. W. Brown, K. Lindenberg, and Bruce J. West, Phys. Rev. B **37**, 2946 (1988).

⁵V. M. Kenkre and D. K. Campbell, Phys. Rev. B **34**, 4959 (1986).

⁶V. M. Kenkre and G. P. Tsironis, Phys. Rev. B **35**, 1473 (1987).

⁷V. M. Kenkre, G. P. Tsironis, and D. K. Campbell, in *Nonlinearity in Condensed Matter*, edited by A. R. Bishop, D. K.

- Campbell, P. Kumar, and S. E. Trullinger (Springer-Verlag, Berlin, 1987).
- ⁸G. P. Tsironis and V. M. Kenkre, *Phys. Lett. A* **127**, 209 (1988).
- ⁹A. S. Davydov, *Solitons in Molecular Systems* (Reidel, Dordrecht, 1985).
- ¹⁰J. M. Hyman, D. W. McLaughlin, and A. C. Scott, *Physica D* **3**, 28 (1981).
- ¹¹M. Toda, *Theory of Nonlinear Lattices* (Springer-Verlag, Berlin, 1981).
- ¹²R. Zwanzig, in *Lectures in Theoretical Physics*, edited by W. Brittin, B. Downs, and J. Down (Interscience, New York, 1961), Vol. III.
- ¹³S. Nakajima, *Prog. Theor. Phys.* **20**, 948 (1958).
- ¹⁴H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Mechanics*, (Springer-Verlag, Berlin, 1982).
- ¹⁵V. M. Kenkre and P. Reineker, in *Exciton Dynamics in Molecular Crystals and Aggregates*, edited by G. Höher (Springer-Verlag, Berlin, 1982).
- ¹⁶V. M. Kenkre, *J. Stat. Phys.* **19**, 333 (1978).
- ¹⁷L. Cruzeiro-Hansson, P. L. Christiansen, and J. N. Elgin, *Phys. Rev. B* **37**, 7896 (1988).
- ¹⁸V. M. Kenkre, *Phys. Lett.* **65A**, 391 (1978).
- ¹⁹R. J. Silbey, *Ann. Rev. Phys. Chem.* **27**, 203 (1976).
- ²⁰V. M. Kenkre and R. S. Knox, *Phys. Rev. Lett.* **33**, 803 (1974).
- ²¹V. M. Kenkre and H.-L. Wu (unpublished); see also V. M. Kenkre, in *Disorder and Nonlinearity*, Los Alamos, 1988, edited by A. Bishop, D. K. Campbell, and S. Pnevmatikos (Springer-Verlag, Berlin, to be published).