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Self-trapping and time evolution in some spatially extended quantum nonlinear systems: Exact solutions

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We present exact analytical solutions of the discrete nonlinear Schrödinger equation for N-site systems by generalizing methods employed previously for the quantum nonlinear dimer and trimer. The transition from localized to delocalized states is markedly different from that in the dimer. A transition, for which there is no dimer analog, occurs in which an initial excitation that is partially localized over a group of sites is found to be partially localized over these same sites or over a different group of sites depending on the strength of the nonlinearity and the asymmetry of the lattice.

I. INTRODUCTION

The discrete nonlinear Schrödinger equation that will be considered in this paper is

$$\frac{dc_m}{dt} = -iV \sum_n{}' c_n + i\chi |c_m|^2 c_m , \tag{1.1}$$

wherein c_m is the amplitude for the system to be in state $|m\rangle$, V is the intersite matrix element describing the linear evolution among the states $|m\rangle$, χ is the nonlinearity which measures the lowering of the site energy due to polaronic effects when the quasiparticle occupies site m, and the prime on the sum indicates that the $n=m$ term is excluded. The manner in which (1.1) differs from the usual form of the discrete nonlinear Schrödinger equation[1-12] is that the site-to-site motion term in (1.1) connects *all* sites in the system in contrast to sites within a small subset such as a nearest-neighbor group. A possible realization of such an N-site system is hydrogen in metals.[13] Some of the hydrogen ions in metal-hydrides get trapped at the interstices near an impurity, such as oxygen, due to the strains resulting from the distortion of the lattice by the impurity. The resulting proton dynamics among the interstices surrounding the impurity should display quantum effects, since the proton is light, and polaron effects, due to strong interstitial-phonon interactions.

In this paper, we present some exact solutions that we obtained[14-16] in the analysis of this system, and comment on the nature of the self-trapping which is particular to it. In a forthcoming paper we describe the application of this analysis to specific experiments.

In Sec. II we convert (1.1) into the corresponding equation obeyed by the density-matrix elements ρ_{mn}, introduce a key quantity $p(t)$ which is natural and convenient for the description of the quasiparticle motion in the present system, and obtain from the density-matrix equation, a closed equation for $p(t)$. The equation is valid for localized initial conditions and a class of more general but symmetric initial conditions. In Sec. III we solve the p equation exactly in terms of elliptic functions and obtain thereby a generalization of the dimer[1-12] and trimer[14] solutions. Particular cases and some extensions are treated in Sec. IV. From the time-dependent solutions we also obtain the stationary states given by Eilbeck, Lomdahl, and Scott.[17] In Sec. V we present some numerical results for the average values around which the probabilities oscillate. A class of complex initial conditions is considered in the Appendix.

II. DERIVATION OF *p* EQUATION

It is straightforward to convert the discrete nonlinear Schrödinger equation (1.1) into the corresponding Liouville-Von Neumann equation for $\rho_{mm} = c_n^* c_m$

$$\frac{d\rho_{mn}(t)}{dt} = -iV \sum_s (\rho_{\mathrm{sn}} - \rho_{ms}) + i\chi(\rho_{mm} - \rho_{nn})\rho_{mn} . \tag{2.1}$$

We will be considering an N-site system with initial conditions for which the excitation is either localized on a single site, partially localized over a group of identical sites (m_A in number), or partially localized over these sites and over a different group of identical sites ($m_B = N - m_A$ in number). Specifically, these real initial conditions are expressed as

$$c_m(t=0) = \begin{Bmatrix} |c_{A,0}| \\ s|c_{B,0}| \end{Bmatrix} \quad \text{for } m \text{ labeling a site of type } \begin{Bmatrix} A \\ B \end{Bmatrix} , \tag{2.2}$$

wherein, the zero subscript indicates the $t=0$ value. The initial amplitudes for the excitation to be at any of the type-B sites can be either in phase ($s=+1$) or out of phase ($s=-1$) with respect to the amplitude on the type-A sites. Symmetry ensures that the amplitudes for each of the type-A sites will have the same time evolution. The amplitudes for each of the type-B sites will also have the same time evolution, but different from that of the type-A sites. In the case of a tetramer, for example, these initial conditions include localized initial conditions $\{c_{1,0}=1,\ c_{2,0}=c_{3,0}=c_{4,0}=0\}$, as well as the partially localized initial conditions $\{c_{1,0}=c_{2,0}=c_{3,0}=\frac{1}{3},\ c_{4,0}=0\}$, and $\{c_{1,0}=\frac{13}{14},\ c_{2,0}=c_{3,0}=c_{4,0}=-\frac{3}{14}\}$. A solution for a restricted class of complex initial conditions which includes those in (2.2) is presented in the Appendix.

For the analysis of the dimer[1-12] and trimer[14] it was convenient to introduce the probability differences $p=\rho_{11}-\rho_{22}$, and $p=\rho_{11}-2\rho_{22}$, respectively. Here, we introduce a natural generalization of these probability differences:

$$p=m_A\rho_{AA}-m_B\rho_{BB} \ . \tag{2.3}$$

Whether there is a single site of type A or a group of them, when the excitation is equally distributed over the A sites, the site occupation probabilities for these sites are simply $1/m_A$, and the probability difference is 1. Similarly, it is -1 for an excitation that is equally distributed over the B sites. The probability difference is $(m_A-m_B)/N$ for a delocalized excitation, and is zero when half of the probability is distributed over the A sites (the remaining half being distributed over the B sites).

The system of coupled equations in (2.1) can now be recast into three coupled equations for p and two other variables, q and r, whose definitions are

$$q=i\sqrt{m_Am_B}(\rho_{AB}-\rho_{BA}) \ , \tag{2.4}$$

$$r=\sqrt{m_Am_B}(\rho_{AB}+\rho_{BA}) \ . \tag{2.5}$$

This choice of p, q, and r is analogous to those used in the dimer[1] and trimer[14] and satisfies

$$p^2+q^2+r^2=1 \ .$$

The coupled equations in p, q, and r are simply

$$\frac{dp}{dt}=2V\sqrt{m_Am_B}q \ , \tag{2.6}$$

$$\frac{dq}{dt}=-2V\sqrt{m_Am_B}p+\left[\frac{(m_A-m_B)(\chi+2m_Am_BV)-N\chi p}{2m_Am_B}\right]r \ , \tag{2.7}$$

$$\frac{dr}{dt}=-\left[\frac{(m_A-m_B)(\chi+2m_Am_BV)-N\chi p}{2m_Am_B}\right]q \ . \tag{2.8}$$

The initial conditions expressed in (2.2) can be expressed in terms of elements of the density matrix, or in terms of the initial values of p, q, and r.

$$\begin{aligned}\rho_{AA,0}&=c_{A,0}^2=\tfrac{1}{2}(1+p_0)/m_A \ ,\\ \rho_{BB,0}&=c_{B,0}^2=(1-m_Ac_{1,0}^2)/m_B=\tfrac{1}{2}(1-p_0)/m_B \ ,\end{aligned} \tag{2.9}$$

$$\rho_{AB,0}=\rho_{BA,0}=c_{A,0}c_{B,0}=s\sqrt{(1-p_0^2)/4m_Am_B} \ , \tag{2.10}$$

$$p_0=2m_Ac_{A,0}^2-1, \quad q_0=0, \quad r_0=s\sqrt{1-p_0^2} \ . \tag{2.11}$$

As with the c's the zero subscripts denote the $t=0$ values. Since $q_0=0$, we see from (2.6) that the initial value of dp/dt is zero. This is the case, because we are considering real initial conditions.

Substituting the solution of (2.8) into (2.7), and substituting the resulting expression into the time derivative of (2.6), we obtain

$$\frac{d^2p}{du^2}=-2\gamma_0-6\gamma_1p-6\gamma_2p^2-2\gamma_3p^3 \ . \tag{2.12}$$

The γ's in (2.12) are given by

$$\gamma_0=\tfrac{1}{2}\eta(2k_0+1)\{[k_0p_0-\eta(2k_0+1)]p_0-r_0\sqrt{1-\eta^2}\} \ , \tag{2.13}$$

$$\gamma_1=\tfrac{1}{6}\{(1-\eta^2)-2k_0(k_0p_0^2-r_0\sqrt{1-\eta^2})+\eta(2k_0+1)[2k_0p_0+\eta(2k_0+1)]\} \ , \tag{2.14}$$

$$\gamma_2=-\tfrac{1}{2}\eta k_0(2k_0+1) \ , \tag{2.15}$$

$$\gamma_3=k_0^2 \ , \tag{2.16}$$

and the three dimensionless quantities u, η, and k_0,

$$u=NVt, \quad \eta=\frac{m_A-m_B}{N}, \quad k_0=\frac{\chi}{N^2V(1-\eta^2)} \ , \tag{2.17}$$

have been introduced. The relative strengths of the nonlinear and linear terms in the discrete nonlinear Schrödinger equation is represented by k_0, and η is a measure of asymmetry in the number of sites in the two groups of sites and has the range $|\eta|\le(N-2)/N<1$.

The closed evolution equation for p shown in Eq. (2.12) has in its right-hand side all non-negative powers of p up to the third power. In this feature, it is similar to the evolution equation for a nondegenerate two-site system.[18]

III. SOLUTION OF p EQUATION

Using the standard procedure involved in the so-called energy method employed in classical mechanics, we multiply (2.12) by dp/du to obtain

$$\int_{(dp/du)_0}^{dp/du}d[dp/du)^2]=-4\int_{p_0}^{p}(\gamma_0+3\gamma_1p+3\gamma_2p^2+\gamma_0p^3)dp \ . \tag{3.1}$$

Performing the integration and remembering that the initial value of dp/du is zero yields

$$\left[\frac{dp}{du}\right]^2=U(p_0)-U(p) \ , \tag{3.2}$$

wherein, the potential U is given by

$$U(p)=4\gamma_0p+6\gamma_1p^2+4\gamma_2p^3+\gamma_3p^4 \ . \tag{3.3}$$

Expanding $(dp/du)^2$ about p_0 and using the change of variable

$$\sigma=-\frac{1}{4}\left[\frac{U'(p_0)}{p-p_0}+\frac{U''(p_0)}{6}\right] \ , \tag{3.4}$$

in which the primes indicate differentiation with respect to p, (3.2) becomes

$$\left[\frac{d\sigma}{du}\right]^2 = 4\sigma^3 - g_2\sigma - g_3 \ . \tag{3.5}$$

The coefficients g_2 and g_3 are related to the γ's and the potential by

$$g_2 = 3\gamma_1^2 - 4\gamma_2\gamma_0 - \gamma_3 U(p_0) \ , \tag{3.6}$$

$$g_3 = \gamma_1^3 + \gamma_3\gamma_0^2 - 2\gamma_2\gamma_1\gamma_0 + (\gamma_3\gamma_1 - \gamma_2^2)U(p_0) \ , \tag{3.7}$$

and, thus, are functions of p_0, k_0, η, and s.

The solution of (3.5) is the Weierstrassian elliptic function $\wp(u;g_2,g_3)$. Substituting this into (3.4) gives the solution for the probability difference.

$$p(u) = p_0 - \frac{6U'(p_0)}{24\wp(u;g_2,g_3) + U''(p_0)} \ . \tag{3.8}$$

This is similar to a solution obtained for a quite different physical system, namely the nondegenerate, nonlinear dimer.[18] The site occupation probabilities follow directly from p

$$\rho_{nn} = \begin{Bmatrix} (1+p)/(2m_A) \\ (1-p)/(2m_B) \end{Bmatrix} \quad \text{for } n \text{ labeling a site of type } \begin{Bmatrix} A \\ B \end{Bmatrix} \ . \tag{3.9}$$

The probability difference in (3.8) is the primary result of this section. It can also be expressed in terms of Jacobian elliptic functions by employing the standard relationships[19] between them. One begins with finding the discriminant Δ and the three roots e_i from the invariants g_2 and g_3.

$$\Delta = g_2^3 - 27g_3^2 \ , \tag{3.10}$$

$$4z^3 - g_2 z - g_3 = 0 = 4(z-e_1)(z-e_2)(z-e_3) \ . \tag{3.11}$$

For those values of g_2 and g_3 that result in a positive discriminant, the three real roots in (3.11) are

$$\begin{aligned} e_1 &= \sqrt{g_2/3}\cos\phi \ , \\ e_2 &= -\sqrt{g_2/12}(\cos\phi - \sqrt{3}\sin\phi) \ , \\ e_3 &= -\sqrt{g_2/12}(\cos\phi + \sqrt{3}\sin\phi) \\ \phi &= \frac{1}{3}\arccos\sqrt{27g_3^2/g_2^3} \ , \end{aligned} \tag{3.12}$$

and the Weierstrassian elliptic function takes the form

$$\begin{aligned} \wp(u) &= e_3 + \frac{e_1 - e_3}{\mathrm{sn}^2(u\sqrt{e_1 - e_3}, k_1)} \ , \\ k_1^2 &= \frac{e_2 - e_3}{e_1 - e_3} \ . \end{aligned} \tag{3.13}$$

If the discriminant is negative, there is one real root (usually taken to be e_2), a complex conjugate pair of roots (e_1 and e_3), and

$$\begin{aligned} e_2 &= \tfrac{1}{2}[(g_3 + \sqrt{-\Delta/27})^{1/3} + (g_3 - \sqrt{-\Delta/27})^{1/3}] \ , \\ H^2 &= 3e_2^2 - \tfrac{1}{4}g_2 \ , \end{aligned} \tag{3.14}$$

$$\wp(u) = e_2 + H\frac{1 + \mathrm{cn}(2u\sqrt{H}, k_2)}{1 - \mathrm{cn}(2u\sqrt{H}, k_2)}, \quad k_2^2 = \frac{1}{2} - \frac{3}{4}\frac{e_2}{H} \ . \tag{3.15}$$

When the discriminant is zero, the Weierstrassian elliptic function takes on simple trigonometric forms.[19]

IV. PARTICULAR CASES AND EXTENSIONS

Substituting (2.13)–(2.16) into (3.6)–(3.7), the discriminant in (3.10) can be factored as

$$\Delta = \tfrac{1}{4}k_0^2[U'(p_0)]^2 O[k_0^4] \ , \tag{4.1}$$

$$U'(p_0) = 2\sqrt{1-\eta^2}\{p_0\sqrt{1-\eta^2} + r_0[2k_0p_0 - \eta(2k_0+1)]\} \ , \tag{4.2}$$

wherein the last term of Δ, of order k_0^4, has simple factors only in very special cases (e.g., when $p_0 = 1$). We see that for the linear N-mer ($k_0 = 0$) and for situations where the initial slope of the potential is zero, the discriminant is zero. These are two of the special cases treated in detail below.

A. Zero nonlinearity

When there is no nonlinear term in the discrete nonlinear Schrödinger equation, we see from (2.15)–(2.17) and (4.1) that k_0, γ_2, γ_3, and Δ are all zero. In this case, (3.3), (3.6), (3.7), and (3.12) reduce to

$$g_2 = \tfrac{1}{12}, \quad g_3 = \tfrac{1}{216}, \quad \{e_i\} = \{\tfrac{1}{6}, \tfrac{-1}{12}, \tfrac{-1}{12}\} \ ,$$

$$U'(p_0) = 2\sqrt{1-\eta^2}[p_0\sqrt{1-\eta^2} + r_0(2k_0p_0 - \eta)] \ , \tag{4.3}$$

$$U''(p_0) = 2 \ ,$$

the probability difference is

$$p(u) = p_0 - 2\sqrt{1-\eta^2}(p_0\sqrt{1-\eta^2} - \eta r_0)\sin^2(\tfrac{1}{2}u) \ , \tag{4.4}$$

and the time-averaged probability difference for zero nonlinearity is simply

$$\langle p \rangle = \eta(\eta p_0 + s\sqrt{1-p_0^2}\sqrt{1-\eta^2}) \ . \tag{4.5}$$

When the initial excitation is only distributed over the A sites, the initial value of p is 1, and the average probability difference is η^2. When there are fewer A sites than B sites, η is less than zero, the average probability difference for zero nonlinearity is greater than η, and the excitation is partially localized on the A sites. Conversely, when m_A is greater than m_B, η is greater than zero (but always less than 1), the average probability difference for zero nonlinearity is less than η, and the excitation is partially localized on the B sites.

B. Stationary states

For $U'(p=p_0)=0$, we see from (4.1) that $\Delta = 0$, and from (3.8) that $p = p_0$ for all time. That is, the system finds itself in a stationary state. Requiring $U'(p=p_0)=0$ gives two solutions: $p_0=\eta, s=+1$, independent of k_0; and

$$k_0=k_{0,\mathrm{ss}}=\frac{\eta\sqrt{1-p_0^2}-sp_0\sqrt{1-\eta^2}}{2(p_0-\eta)\sqrt{1-p_0^2}} . \tag{4.6}$$

Figure 1 shows $k_{0,\mathrm{ss}}$ as a function of p_0 for two particular values of $\eta(+\frac{1}{3}$ and $-\frac{1}{2})$ for both in-phase and out-of-phase stationary states. The explicit form of $k_{0,\mathrm{ss}}$ in (4.6) is equivalent to the expression given in Sec. 3.2 and the parametric forms given in Secs. 3.3 and 3.4i of Ref. 17 with their $N=1$, $\epsilon=-V\gamma=\chi$, and n equal to 2, 3, and 4, respectively. Since the reduced system (the general system subject to specific initial conditions) involves explicit initial conditions, a stationary state of the reduced system need not necessarily be a stationary state of the total system. This is so because the initial conditions assumed need not be compatible with the stationary states of the total system. We find, however, that the stationary states of the reduced system are stationary states of the total system.

The site occupation probabilities ρ_{mm} for stationary states of the total system specified by (2.1) are time independent. For the stationary states, (2.1) gives us the requirement

$$\sum_s (\rho_{sm}-\rho_{ms})=0 , \tag{4.7}$$

for all m and time. For the reduced system we have considered, the left-hand side of (4.7) is

$$\sum_s (\rho_{sm}-\rho_{ms})=\begin{Bmatrix} m_B(\rho_{BA}-\rho_{AB}) \\ m_A(\rho_{AB}-\rho_{BA}) \end{Bmatrix}$$

$$\text{for } m \text{ labeling a site of type} \begin{Bmatrix} A \\ B \end{Bmatrix} . \tag{4.8}$$

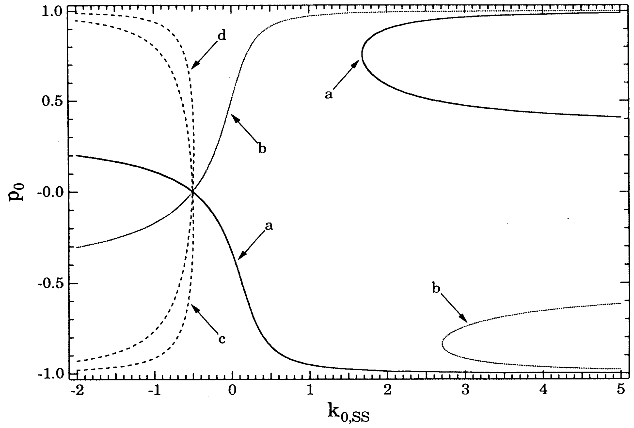

FIG. 1. Variation of the stationary-state nonlinearity parameter with the initial probability difference for a degenerate nonlinear N-mer as given in (4.6) for particular cases. Curves a and c are for a trimer $(\eta=\frac{1}{3}, m_A=2, m_B=1)$ with out-of-phase and in-phase initial conditions, respectively. Similarly, curves b and d are for a tetramer $(\eta=-\frac{1}{4}, m_A=1, m_B=3)$.

For a stationary state of the reduced system $dp/dt=0$, and we see from (2.4) and (2.6) that $\rho_{AB}-\rho_{BA}=0$. The stationary states of the reduced system, thus, satisfy (4.7) and are stationary states of the general system.

C. Localized initial conditions

When the initial amplitude is equally distributed over the A sites, $p_0=1$, and the last term of Δ in (4.1) can be factored as

$$-(1-\eta^2)[(1-\eta)k_0+1][16\eta(1-\eta^2)k_0^3-8\eta(1-\eta)$$
$$\times(1+4\eta)k_0^2-(16\eta^3-8\eta^2-11\eta+1)k_0-1] . \tag{4.9}$$

For $k_0=-1/(1-\eta)$ the first term in brackets in (4.9) is zero, as is Δ. For this special case, (3.3), (3.6)–(3.7), and (3.12) simplify to

$$\begin{gathered} g_2=\tfrac{1}{12}(1+2\eta)^2, \quad g_3=\tfrac{-1}{216}(1+2\eta)^3 , \\ \{e_1\}=\left\{\frac{1+2\eta}{12},\frac{1+2\eta}{12},-\frac{1+2\eta}{6}\right\} , \\ U'(p_0)=2(1-\eta^2), \quad U''(p_0)=2(5+4\eta). \end{gathered} \tag{4.10}$$

With η in the range $-\frac{1}{2}\leq\eta<1$, g_3 is negative, the probability difference is

$$p(u)=\frac{(1+2\eta)+2\eta(1+\eta)\sinh^2(\frac{1}{2}u\sqrt{1+2\eta})}{(1+2\eta)+2(1+\eta)\sinh^2(\frac{1}{2}u\sqrt{1+2\eta})} , \tag{4.11}$$

and the time-averaged probability difference is

$$\langle p\rangle=\eta \tag{4.12}$$

With η in the range $-1<\eta\leq-\frac{1}{2}$, g_3 is positive, the probability difference is

$$p(u)=\frac{-(1+2\eta)+2\eta(1+\eta)\sin^2(\frac{1}{2}u\sqrt{-1-2\eta})}{-(1+2\eta)+2(1+\eta)\sin^2(\frac{1}{2}u\sqrt{-1-2\eta})} , \tag{4.13}$$

and the time-averaged probability difference is

$$\langle p\rangle=\eta+(1+\eta)\sqrt{-1-2\eta} . \tag{4.14}$$

For initial conditions which are completely localized on a single site $(m_A=1, m_B=N-1)$, η in (4.12) and (4.14) takes the particular value $-(N-2)/N$.

D. Reduction to a pseudodimer

When there are an even number of sites in the N-mer and they are equally divided between the two sites types, η is zero. For this case, we see from (2.13) and (2.15) that the coefficients of the even powers of p in (2.12) are zero. The resulting p equation is similar to that of the dimer[3-7] in that only odd powers of p are present. In this pseudodimer case, the coefficients reduce to

$$\begin{gathered} \gamma_0=\gamma_2=0 , \\ \gamma_1=\tfrac{1}{6}(1-2k_0^2p_0^2+2sk_0\sqrt{1-p_0^2}), \quad \gamma_3=k_0^2 , \end{gathered} \tag{4.15}$$

and we see that the terms that remain in the p equation are either quadratic in k_0 or linear in sk_0. Thus, we need only consider $k_0>0$, and $s=\pm 1$.

For large nonlinearity, $k_0>(1+s\sqrt{1-p_0^2})/p_0^2$, the real roots in (3.11) simplify to

$$\{e_i\}=\{-\tfrac{1}{2}[\gamma_1-\sqrt{-\gamma_3 U(p_0)}]\,,\; -\tfrac{1}{2}[\gamma_1+\sqrt{-\gamma_3 U(p_0)}],\gamma_1\}\;. \tag{4.16}$$

Upon substituting (4.15), (4.16), and (3.13) into (3.8) we obtain

$$p=p_0\frac{1-k_1\mathrm{sn}^2(\sqrt{e_1-e_3}\,u,k_1)}{1+k_1\mathrm{sn}^2(\sqrt{e_1-e_3}\,u,k_1)}\;, \tag{4.17}$$

wherein,

$$k_1=\frac{2k_0^2p_0^2-2k_0p_0(k_0^2p_0^2-1-2k_0s\sqrt{1-p_0^2}\,)^{1/2}}{1+2k_0s\sqrt{1-p_0^2}}-1\;,$$
$$\sqrt{e_1-e_3}=\tfrac{1}{2}[k_0p_0+(k_0^2p_0^2-1-2k_0s\sqrt{1-p_0^2}\,)^{1/2}]\;. \tag{4.18}$$

Employing the descending Landen or Gauss transformation, the probability difference for a pseudodimer with large nonlinearity, (4.17), simplifies to

$$p=p_0 dn\,(k_0p_0u,1/k_{\mathrm{pd}})\;,$$
$$k_{\mathrm{pd}}^2=\frac{k_0^2p_0^2}{1+2k_0s\sqrt{1-p_0^2}}\;. \tag{4.19}$$

For small nonlinearity, $0<k_0<(1+s\sqrt{1-p_0^2}\,)/p_0^2$, there is one real root and a complex conjugate pair of roots to (3.11). In this situation, the expressions in (3.14) simplify to

$$e_2=\gamma_1,\quad H=\tfrac{1}{2}(\tfrac{1}{2}+k_0s\sqrt{1-p_0^2}\,)\;, \tag{4.20}$$

and the k_2 in (3.15) reduces to k_{pd}. Substituting (4.15), (4.20), and (3.15) into (3.8) we obtain the probability difference for a pseudodimer with small nonlinearity as

$$p=p_0\mathrm{cn}(uk_0p_0/k_{\mathrm{pd}},k_{\mathrm{pd}})\;. \tag{4.21}$$

The N dependence of the pseudodimer results in (4.19) and (4.21) arises from the N dependence of k_0, which also appears in k_{pd}. For $N=2$, these pseudodimer expressions are identical to those for the dimer.[6]

E. Extensions to other three-and four-site systems

Since the amplitudes for the A sites are equal for all time, the intersite matrix element connecting these sites is of no importance and can be set equal to zero. The same is true for those connecting the B sites to one another. The solution in Sec. III applied to the trimer ring ($\eta=\pm\frac{1}{3}$), thus, is also the solution for a trimer chain (three-site system without periodic boundary conditions) subject to initial conditions in which the two end sites have equal amplitudes. Similarly, the tetramer for $\eta=\pm\frac{1}{2}$ reduces to a two-dimensional star shape, and for $\eta=0$ to a four-site ring with alternating A and B sites. The breaking of these "bonds" in the trimer and tetramer is shown in Fig. 2.

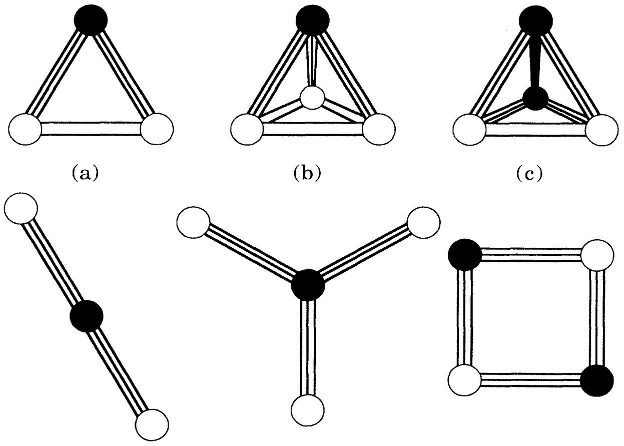

FIG. 2. Breaking of bonds between equivalent sites producing (a) a trimer chain from a trimer ring ($\eta=\pm\frac{1}{3}$), (b) a tetramer star from a tetramer tetrahedron with $\eta=-\pm\frac{1}{2}$, and (c) a tetramer ring with alternating site types from a tetramer tetrahedron with $\eta=0$ (pseudodimer).

V. MEAN VALUES

In Secs. IV A–IV C are analytical expressions for the time-averaged probability difference for some special cases. Here, numerical results are presented for the same quantity, as a function of the nonlinearity parameter k_0 for various initial conditions, and lattice asymmetries η. From the discussion following (2.3), a delocalized excitation is indicated by $p=\eta$, an excitation completely on the A sites has $p=1$, and an excitation completely on the B sites is indicated by $p=-1$. When the probability difference is in the range $\eta<p<1$, the excitation is partially localized on the A sites, whereas it is partially localized on the B sites for p in the range $-1<p<\eta$. If half of the probability is distributed over the A sites, the probability difference is zero.

The analysis presented thus far is applicable to systems for which all sites have the same site-to-site interaction. If this is to be interpreted as spatially nearest neighbors in at most three spatial dimensions, we can consider a one-dimensional dimer, a two-dimensional trimer ring, and a three-dimensional tetramer tetrahedron. In these situations, the lattice asymmetry parameter η takes on the following values:

η		m_A		
		1	2	3
m_B	1	0	$\frac{1}{3}$	$\frac{1}{2}$
	2	$-\frac{1}{3}$	0	
	3	$-\frac{1}{2}$		

In Figs. 3–8, we present the particular cases of the N-mer listed above. These include the previously found dimer[6] and trimer[14] (only $\eta=-\frac{1}{3}$) results, which are displayed for comparison with our new results. The $\eta=0$ curve in these figures is applicable to the dimer and the tetramer when it takes the form of a pseudodimer ($m_A=m_B$). Once the dimensionless ratio χ/V is scaled by N and η, as indicated in (2.17), to become k_0 all pseudodimers have identical behaviors. Thus, it is sufficient to make comparisons to the dimer. Conclusions drawn from such comparisons apply to all pseudodimers.

The average probability difference for an initial condition which is localized on a single site ($m_A=1$) for the dimer ($m_B=1,\eta=0$), trimer ($m_B=2,\eta=-\frac{1}{3}$), and tetramer ($m_B=3,\eta=-\frac{1}{2}$) is displayed in Fig. 3. In all three cases we see that there are ranges of values of the nonlinearity parameter for which the average probability difference is greater than η and, therefore, the excitation is self-trapped on the initially occupied site. We also notice that only the dimer displays a range of nonlinearity parameter for which delocalized states ($\langle p\rangle=\eta$) exist. For the trimer and tetramer, only a single value of k_0 results in delocalized states. The local-to-delocal transition found previously for the dimer[3] is reduced to a single point for the trimer and tetramer. The unique value of the nonlinearity parameter for which delocalized states arise was found in Sec. IV C to be $-1/(1-\eta)$, as was the average probability difference. As the nonlinearity parameter is increased or decreased from this value, the excitation is partially localized about the initial site. Even for zero nonlinearity, an initially localized excitation on a trimer or tetramer is partially localized about the initial site with $\langle p\rangle=\eta^2>\eta$.

Figure 4 displays the average probability difference for an initial condition in which the probability is equally distributed over all but one site ($m_B=1$) for the dimer ($m_A=1,\eta=0$), trimer ($m_A=2,\eta=\frac{1}{3}$), and tetramer ($m_A=3,\eta=\frac{1}{2}$). The dimer results are, of course, identical to those shown in Fig. 3. For the trimer and the tetramer, we observe a range of values of the nonlinearity parameter for which the probability difference is *less* than η. That is, starting with an excitation that is partially localized over a group of sites, the resulting state is partially localized on the initially *unoccupied* site; the excitation has migrated before being self-trapped. When the magnitude of k_0 is large enough, the average probability difference is greater than η, and the excitation remains partially localized on the initially *occupied* sites; the excitation is self-trapped without having migrated.

As a specific case of this transition, consider the tetramer with the initial site occupation probabilities

$$\{\rho_{11,0},\rho_{22,0},\rho_{33,0},\rho_{44,0}\}=\{\tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3},0\} .$$

There are two values of k_0, about 0.2 and -1.5, for

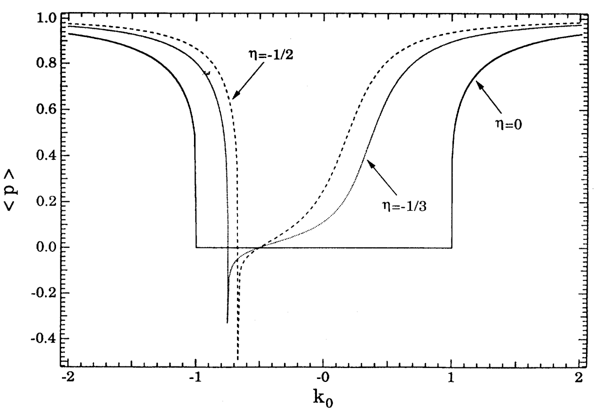

FIG. 3. Dependence of the average probability difference on the nonlinearity parameter for degenerate nonlinear N-mers with the initial amplitude localized on a single site ($p_0=1,m_A=1$) for the dimer $\{m_B=1,\eta=0\}$, trimer $\{m_B=2,\eta=-\frac{1}{3}\}$, and tetramer: $\{m_B=3,\eta=-\frac{1}{2}\}$.

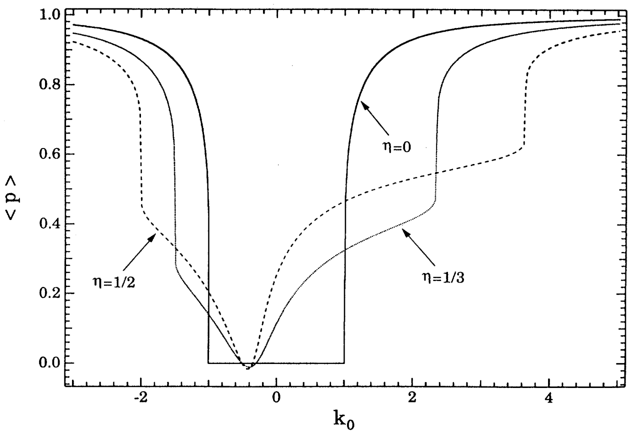

FIG. 4. Similar to Fig. 3, but with the initial amplitude equally distributed over all but a single site ($p_0=1,m_B=1$) for the dimer $\{m_A=1,\eta=0\}$, trimer $\{m_A=2,\eta=\frac{1}{3}\}$, and tetramer: $\{m_A=3,\eta=\frac{1}{2}\}$.

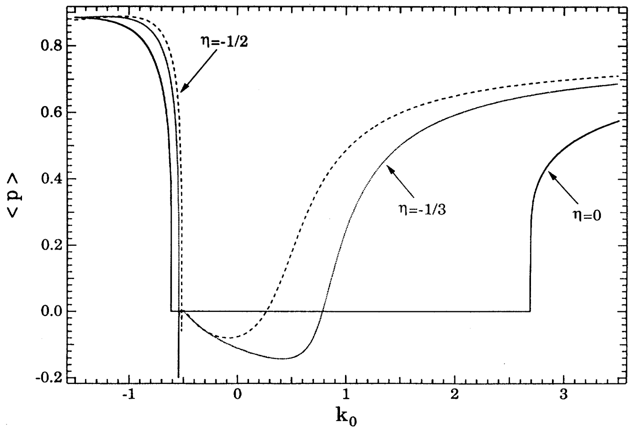

FIG. 5. Dependence of the average probability difference on the nonlinearity parameter for degenerate nonlinear N-mers with the initial amplitude partially localized ($p_0=\frac{7}{9}$) on a single A site ($\eta\leq 0$) and with the initial amplitude on the B sites in phase ($s=+1$) with that on the A sites. The initial amplitudes $\{c_{m,0}\}$ are: $\{\frac{2}{3}\sqrt{2},\frac{1}{3}\}$ for the dimer, $\{\frac{2}{3}\sqrt{2},\frac{1}{6}\sqrt{2},\frac{1}{6}\sqrt{2}\}$ for the trimer, and $\{\frac{2}{3}\sqrt{2},\frac{1}{9}\sqrt{3},\frac{1}{9}\sqrt{3},\frac{1}{9}\sqrt{3}\}$ for the tetramer.

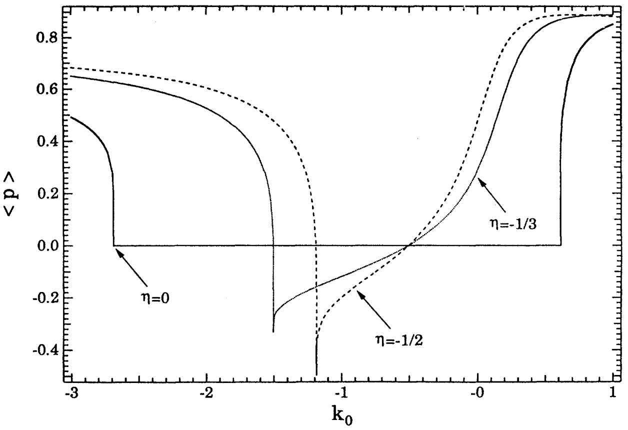

FIG. 6. Similar to Fig. 5, but with the initial amplitude on the B sites out of phase ($s=-1$) with that on the A sites. The initial amplitudes $\{c_{m,0}\}$ are: $\{\frac{2}{3}\sqrt{2},\frac{-1}{3}\}$ for the dimer, $\{\frac{2}{3}\sqrt{2}\frac{-1}{6}\sqrt{2},\frac{-1}{6}\sqrt{2}\}$ for the trimer, and $\{\frac{2}{3}\sqrt{2},\frac{-1}{9}\sqrt{3},\frac{-1}{9}\sqrt{3},\frac{-1}{9}\sqrt{3}\}$ for the tetramer.

which the average probability difference is $\frac{1}{3}$ and the average site probabilities are

$$\{\langle\rho_{11}\rangle,\langle\rho_{22}\rangle,\langle\rho_{33}\rangle,\langle\rho_{44}\rangle\}=\{\tfrac{2}{9},\tfrac{2}{9},\tfrac{2}{9},\tfrac{1}{3}\}\ .$$

Since $\langle\rho_{44}\rangle$ is greater than $\frac{1}{4}$, the excitation is partially localized on site 4, the initially unoccupied site. More complete localization of the excitation onto the initially unoccupied site is evident when k_0 is $-\frac{1}{2}$. For this situation $\langle p\rangle=0$ and $\{\langle\rho_{nn}\rangle\}=\{\frac{1}{6},\frac{1}{6},\frac{1}{6},\frac{1}{2}\}$. For a narrow range of k_0 (near $k_0=-0.4$), $\langle p\rangle$ is less than zero and $\langle\rho_{44}\rangle$ is greater than $\frac{1}{2}$.

The transition from migratory to nonmigratory self-trapping occurs at the two values of k_0 for which $\langle p\rangle=\eta$. One of these values, $k_0=-1/(1-\eta)$, was found in Sec. IV C. A numerical value for the other can be found by finding the real root of the term in (4.9) that is cubic in k_0.

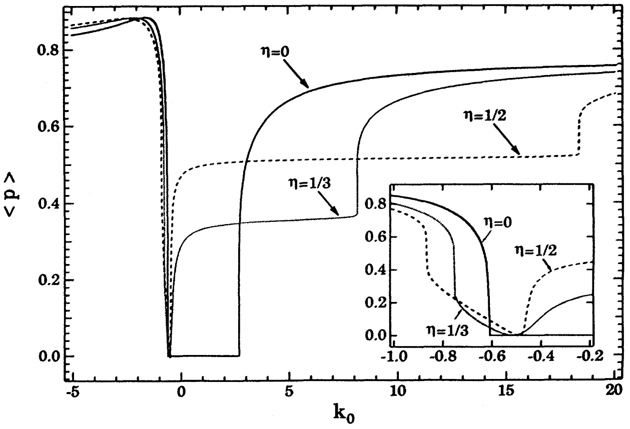

FIG. 7. Similar to Fig. 5, but with the initial amplitude partially localized ($p_0=-\frac{7}{9}$) on all but a single B site ($\eta\geq 0$) and with the initial amplitude on the B site in phase ($s=+1$) with that on the A sites. The initial amplitudes $\{c_{m,0}\}$ are: $\{\frac{2}{3}\sqrt{2},\frac{1}{3}\}$ for the dimer, $\{\frac{2}{3}\sqrt{2},\frac{2}{3}\sqrt{2},\frac{1}{3}\}$ for the trimer, and $\{\frac{2}{9}\sqrt{6},\frac{2}{9}\sqrt{6},\frac{2}{9}\sqrt{6},\frac{1}{3}\}$ for the tetramer. the inset shows the details near $k_0=-0.5$.

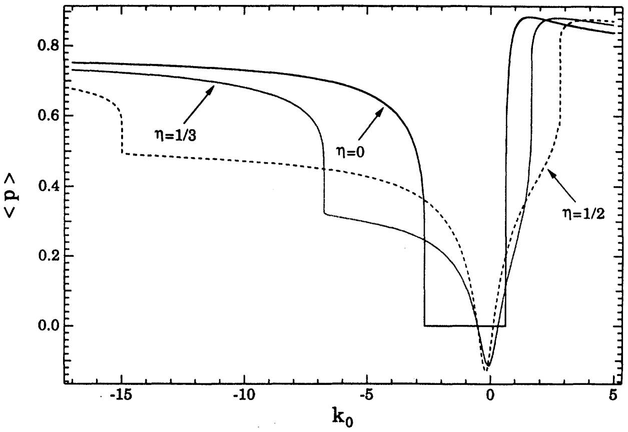

FIG. 8. Similar to Fig. 7, but with the initial amplitude on the B site out of phase ($s=-1$) with that on the A sites. The initial amplitudes $\{c_{m,0}\}$ are: $\{\frac{2}{3}\sqrt{2},\frac{-1}{3}\}$ for the dimer, $\{\frac{2}{3}\sqrt{2},\frac{2}{3}\sqrt{2},\frac{-1}{3}\}$ for the trimer, and $\{\frac{2}{9}\sqrt{6},\frac{2}{9}\sqrt{6},\frac{2}{9}\sqrt{6},\frac{-1}{3}\}$ for the tetramer.

Figures 5–8 display the average probability differences for initial conditions in which the B sites, in addition to the A sites, have nonzero probabilities. For these initial conditions we must specify whether or not the initial amplitudes for the excitation to be on the B sites are in phase ($s=+1$) or out of phase ($s=-1$) with respect to those on the A sites. In comparing Figs. 5 and 6 with Fig. 3, and Figs. 7 and 8 with Fig. 4, the distinguishing features are shifted to larger k_0 for in-phase initial conditions and to smaller k_0 for out-of-phase initial conditions. The width of some features is also changed. The gross behavior of the probability difference, however, is the same in that the regions of migratory and nonmigratory self-trapped, as well as untrapped, states still remain.

All of the curves in Figs. 3–8 pass through the point ($k_0=-\frac{1}{2},\langle p\rangle=0$). For this value of k_0, we see from (2.13), (2.15), and (3.3) that both γ_0 and γ_2 are zero and that the potential $U(p)$ is a symmetric quartic function of p with $U(0)=0$.

$$U(p)=\tfrac{1}{4}p^4+[(1-\eta^2)-\tfrac{1}{2}p_0^2-s\sqrt{1-\eta^2}\sqrt{1-p_0^2}\,]p^2\ . \tag{5.1}$$

When η is in the range $|\eta|<\sqrt{3/4}$ and the initial conditions are out of phase, $U(p_0)$ is always greater than zero, the probability difference oscillates between $+p_0$ and $-p_0$, and the average probability difference is zero. For this range of η and in-phase initial conditions, the probability difference can be confined to one of the troughs in the potential. If p_0 is in the range

$$|p_0|>2[\sqrt{1-\eta^2}-(1-\eta^2)]^{1/2}\ ,$$

$U(p_0)$ is greater than zero, and the average probability difference is again zero. For p_0 outside this range, however, $U(p_0)$ is less than zero, the probability difference oscillates in either the positive or negative trough of the potential, and has a nonzero average probability difference.

A similar situation arises for $|\eta| > \frac{3}{4}$. For this case, in-phase initial conditions give rise to a probability difference that always oscillates in a trough of the potential, whereas, out-of-phase initial conditions does so only for

$$|p_0| > 2[\sqrt{1-\eta^2}-(1-\eta^2)]^{1/2} .$$

For both cases, the critical values of η are found by requiring $U(p=p_0=1)$ to be zero, where as the critical values of p_0 are determined by requiring $U(p_0)$ to be zero for a given η.

VI. DIFFERENCES BETWEEN THE N-MER AND THE DIMER

For the localized and partially localized, real, initial conditions considered thus far, we can draw the following distinctions between the N-mer and the dimer which are independent of the degree of the initial partial localization.

(i) An excitation on a dimer[1-6] or pseudodimer ($\eta=0$) is delocalized (untrapped) for a range of values for χ/V, and becomes self-trapped when the magnitude of χ/V is large enough. The self-trapping is always of the nonmigratory type.

(ii) When the lattice asymmetry favors those sites which have a smaller initial probability ($m_A < m_b, \eta < 0$), an excitation on an N-mer is in a nonmigratory self-trapped state for all but a special value of χ/V. At this special value, the excitation is completely delocalized. The excitation is in a nonmigratory self-trapped state even for zero nonlinearity.

(iii) When the lattice asymmetry favors those sites which have a larger initial probability ($m_A > m_b, \eta > 0$), an excitation on an N-mer may be partially localized on the same sites on which it was partially localized initially (nonmigratory self-trapped), or on the sites which had the smaller initial probabilities (migratory self-trapped). A migratory-to-nonmigratory self-trapping transition takes place for two values of χ/V. At these particular values the excitation is delocalized over all of the sites (untrapped). For values of χ/V which are bounded by these special values, the excitation is in a migratory self-trapped state. For values of χ/V outside of these bounds, the excitation is in a nonmigratory self-trapped state. The excitation is in a migratory self-trapped state even for zero nonlinearity.

VII. CONCLUSIONS

We have found an analytical solution for the time-dependent probability amplitudes of the degenerate, nonlinear N-mer for a class of initial conditions, and have displayed specific results for the trimer and the tetramer. From this solution, we recover the stationary states of the trimer and the tetramer previously found by Eilbeck, Lomdahl, and Scott.[17] Expressions have been found for the average probabilities in special cases, and their dependence on system parameters has been investigated numerically. A new migratory-to-nonmigratory self-trapping transition has been investigated. Through a simple extension of the technique of solution presented here, we have obtained solutions for the trimer chain, the tetramer ring, and the tetramer star for a class of initial conditions.

APPENDIX

This appendix addresses the modifications to the analysis in Secs. II and III that are required to include the following complex initial conditions:

$$c_m(t=0)=\begin{Bmatrix} c_A \\ c_B \end{Bmatrix} \quad \text{for } m \text{ labeling a site of type } \begin{Bmatrix} A \\ B \end{Bmatrix} , \tag{A1}$$

The real initial conditions in (2.2) are a subset of these.

The definitions of p, q, r, and their time derivatives in (2.3)–(2.8) are unchanged. The particular forms for q_0 and r_0 in (2.11) are now given by

$$\begin{aligned} q_0 &= i\sqrt{m_A m_B}(c^*_{B,0}c_{A,0}-c^*_{A,0}c_{B,0}) \\ &= \frac{1}{2V\sqrt{m_A m_B}}\left[\frac{dp}{dt}\right]_0 , \end{aligned} \tag{A2}$$

$$r_0=\sqrt{m_A m_B}(c^*_{B,0}c_{A,0}+c^*_{A,0}c_{B,0})=\sqrt{1-p_0^2-q_0^2} . \tag{A3}$$

The initial conditions, thus, can either be expressed in terms of $c_{A,0}$ and $c_{B,0}$ or p_0 and $(dp/dt)_0$. The p equation, and the definitions of the γ's, u, η, and k_0 in (2.13)–(2.17) do not change. The first real departure from the analysis comes at (3.2). Here, $(dp/dt)_0$ is not zero, so

$$\left[\frac{dp}{du}\right]^2 = \left[\left[\frac{dp}{du}\right]_0\right]^2 + U(p_0) - U(p) = f(p) . \tag{A4}$$

The potential in (A4) is still given by (3.3), and the $(dp/dt)_0$ term has the attributes of an "initial kinetic-energy" term. Rearranging (A4),

$$du = dp/\sqrt{f(p)} , \tag{A5}$$

and defining p_1 to be a real root of $f(p)=0$, the definite integral of (A5) can be written as

$$\begin{aligned} u &= \int_{p_0}^{p} dp/\sqrt{f(p)} \\ &= \int_{p_0}^{p_1} dp/\sqrt{f(p)} + \int_{p_1}^{p} dp/\sqrt{f(p)} . \end{aligned} \tag{A6}$$

Expanding $f(p)$ about p_1 and using the change of variable

$$\sigma = -\frac{1}{4}\left\{\frac{U'(p_1)}{p-p_1}+\frac{U''(p_1)}{6}\right] , \tag{A7}$$

(A6) becomes

$$u-u_0=\int_{\sigma}^{\infty} d\lambda/\sqrt{4\lambda^3-g_2\lambda-g_3}\ , \tag{A8}$$

wherein

$$u_0=-\int_{\sigma_0}^{\infty} d\lambda/\sqrt{4\lambda^3-g_2\lambda-g_3},\quad \sigma_0\equiv\sigma(p=p_0)\ . \tag{A9}$$

$$g_2=3\gamma_1^2-4\gamma_2\gamma_0-\gamma_3 U(p_1)\ , \tag{A10}$$

$$g_3=\gamma_1^3+\gamma_3\gamma_0^2-2\gamma_2\gamma_1\gamma_0+(\gamma_3\gamma_1-\gamma_2^2)U(p_1)\ . \tag{A11}$$

The integral form for the Weierstrassian elliptic function is evident in (A8), and u_0 is an elliptic integral in terms of p_0, $(dp/dt)_0$, k_0, and η. The invariants, g_2 and g_3, differ from those in (3.6) and (3.7) in that the potential is evaluated at p_1 instead of p_0. Inverting (A9) and using (A7) we find

$$p(u)=p_1-\frac{6U'(p_1)}{24\wp(u-u_0;g_2,g_3)+U''(p_1)}\ . \tag{A12}$$

This probability difference is the generalization of the N-mer solution in (3.8) for the complex initial conditions in (A1). When real initial conditions are considered, $(dp/du)_0=0$, and from (A4), p_1, the root of $f(p)=0$, is equal to p_0. Substituting $p_1=p_0$ into (A9) gives $\sigma_0=\infty$, and $u_0=0$. The expression in (A12), thus, reduces to (3.8) for real initial conditions.

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