Bifurcations in resonance widths of an open Bose-Hubbard dimer

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We investigate the structure of resonance widths of a Bose-Hubbard dimer with intersite hopping amplitude k, which is coupled to a continuum at one of the sites with strength γ. Using an effective non-Hermitian Hamiltonian formalism, we show that by varying the on-site interaction term χ the resonances undergo consequent bifurcations. For $\Lambda = k/\gamma \geq 0.5$, the bifurcation points follow a scaling law $\tilde{\chi}_m \equiv \chi_m N/k = f_\Lambda(m - 0.5/\Lambda)$, where N is the number of bosons. For the function f_Λ two different Λ dependences are found around the minimum and maximum bifurcation points.

The interplay of intrinsic dynamics with coupling to the continuum, radiation field, or any other external influence, such as measurement, is an important subject for various branches of modern physics: quantum chaos [1], nanoscale devices [2], quantum optics [3], theory of decoherence, and quantum computing [4] up to nuclear [5], atomic and molecular physics [6] are some of the areas, seemingly far remote from each other, that have boosted research in open systems. These systems are often described within the "effective non-Hermitian Hamiltonian" formalism [5]. The eigenvalues of the effective Hamiltonian are complex $\mathcal{E}_n = E_n - i\Gamma_n/2$, with the nonzero imaginary part, describing the rate with which an eigenstate of the open system (termed resonance state) decays in time due to the coupling to the "outside world."

With the advent of sophisticated techniques for trapping and transporting ultracold atoms, resonance states become an issue also in the context of Bose-Einstein condensates (BEC). Examples include "atom lasers" [7], optical tweezers [8], and magnetic "conveyor belts" [9], as well as microtraps on "atom chips" [10], which were suggested as potential building blocks for quantum-information processing [11]. In this context, the aim is to understand the scattering and decay properties of a condensate leaking out of the trap via tunneling.

The first theoretical investigations of the waveguide scattering of a BEC through a double-barrier potential, acting like a quantum dot for the atoms, reveal intriguing nonlinear effects associated with the internal resonances of the quantum dot [12]. Complementary studies of the decay of a condensate from one open trapping potential were reported in [13–15], while a first attempt to study the current relaxation of an ultracold BEC periodically driven with a standing wave of laser light was performed in [16]. The theoretical approaches used in these studies were based on the nonlinear Gross-Pitaevskii equation describing the mean-field dynamics of the condensate.

However, a full quantum many-body study of decaying properties of a BEC is lacking. If the hopping amplitude between nearby traps is small compared with the excitation energies in higher bands, one can use a Bose-Hubbard Hamiltonian (BHH) to describe the condensate quantum mechanically. This is the simplest nontrivial model that describes interacting bosons on a lattice and incorporates the competition between kinetic and interaction energy of the bosonic system. In this context, the closed two-site system (dimer) has been analyzed thoroughly and many interesting phenomena have been found [17–20,27]. The richness of the results provides a motivation to go beyond the closed dimer and consider new scenarios where even richer behavior should be observed. In this respect, the open quantum dimer promises new exciting opportunities, since the coupling to continuum leads to an interesting interplay with the internal dynamics.

In this paper we address such a scenario and study the resonance linewidths Γ of a BHH coupled to continuum from one of the two sites. One possible realization of this setup is two coupled bosonic traps where tunneling to a continuum is imposed at one site. Another motivation comes from exciton transfer in molecular aggregates in which guest molecules (traps) are introduced interstitially and excitons are captured once they appear inside the sphere of influence of the traps [21]. Using an effective Hamiltonian formalism, we show the appearance of consequent bifurcations in the resonance widths Γ_n as we change the on-site interaction strength χ. The resonances follow a scaling law

$$\tilde{\Gamma}(k,\gamma,N) \equiv \frac{\Lambda}{Nk}\Gamma = \Phi_\Lambda(\tilde{\chi}), \quad \tilde{\chi} = \chi N/k, \qquad (1)$$

where N is the total number of interacting bosons, k the hopping amplitude, γ the coupling to continuum, and $\Lambda \equiv k/\gamma$. In particular, we reveal that if the dimensionless ratio $\Lambda \equiv k/\gamma$ is larger than $\Lambda^* = 0.5$, then for N interacting bosons there are $N/2$ [22] bifurcation points $\chi_m, m=1,\ldots,N/2$ which follow a scaling law

$$\tilde{\chi}_m \equiv \frac{\chi_m N}{k} = f_\Lambda(\mu), \quad \mu \equiv \frac{m - 0.5/\Lambda}{N}, \qquad (2)$$

where f_Λ represent a set of one-parameter scaling functions which depend on Λ. Two different Λ dependences are found for the upper and lower parts of the bifurcation spectrum.

The former is Λ independent and thus universal while for the latter we have

$$\widetilde{\chi}_m/\widetilde{\chi}^* = g(\mu), \quad \widetilde{\chi}^* = \exp(-1.55/\Lambda), \quad (3)$$

where $g(\cdot)$ is a universal (Λ-independent) scaling function. Our results [(1)–(3)] are confirmed numerically and are supported by theoretical arguments.

A usual way to treat the coupling of bound states with continuum is to exclude the continuum degrees of freedom from consideration by the introduction of an effective Hamiltonian H^{eff} acting within the subspace of bound states and implicitly taking into account their interaction with the continuum [5]. In the case of a dimer trap, it is natural to assume that the probability to escape in the continuum is proportional to the number of the bosons located at the site (say the second one) which is coupled to the continuum [23]. Following this line of argumentation we come out with an H^{eff} given by

$$\hat{H}^{\text{eff}} = \frac{\chi}{2}\sum_{i=1}^{2}\hat{n}_i(\hat{n}_i - 1) - k\sum_{i\neq j}\hat{b}_i^\dagger\hat{b}_j - i\gamma\hat{b}_2^\dagger\hat{b}_2, \quad (4)$$

where $\chi = 4\pi\hbar^2 a_s V_{\text{eff}}/m_0$ describes the interaction between two atoms on a single site (V_{eff} is the effective mode volume of each site, m_0 is the atomic mass, and a_s is the s-wave scattering length of atoms which can be either positive or negative and can be controlled experimentally). The operators $\hat{n}_i = \hat{b}_i^\dagger\hat{b}_i$ count the number of bosons at site i; the annihilation and creation operators $\hat{b}_i$ and $\hat{b}_i^\dagger$ obey the canonical commutation relations $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{i,j}$. We note that a similar effective Hamiltonian was used to study a leaking dimer [24] in the presence of pumping or driving light field [25]. The Hamiltonian (4) in the fixed (instantaneous) basis of the eigenstates of $\hat{N} = \Sigma_{i=1}^{2}\hat{n}_i$ reads

$$H_{nm}^{\text{eff}} = \begin{cases} \frac{\chi}{2}[n^2 + (N-n)^2 - N] - i\gamma(N-n), & n = m, \\ -k\sqrt{n(N+1-n)}, & n = m+1, \\ -k\sqrt{(n+1)(N-n)}, & n = m-1, \\ 0, & \text{else.} \end{cases} \quad (5)$$

where $n, m = 0, 1, \ldots, N$. We are interested in its (instantaneous) complex eigenvalues $\mathcal{E}_n = E_n - i\frac{\Gamma_n}{2}$, where E_n and Γ_n are the position and width of the resonances, respectively. The subindex n indicates the number of bosons on the first (nondissipative) site. Accordingly $N-n$ bosons are on the second (dissipative) site. The rank of H^{eff} is related to the number of particles as $\mathcal{N} = N+1$. In our numerical analysis we consider traps with number of particles $N = 10$ up to 500.

To gain some insight in to the parametric evolution of resonance widths, let us first consider the two limiting cases: vanishing interaction $\chi = 0$ and very strong interaction $\chi \gg k$. In the former case one finds that the eigenvalues $\mathcal{E}_n$ of the effective Hamiltonian are given by
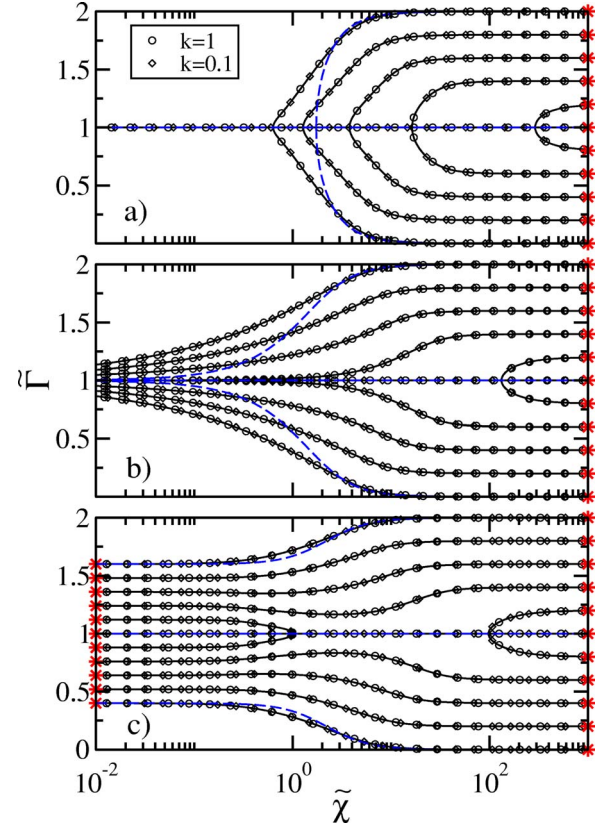

FIG. 1. (Color online) Bifurcation diagram for the rescaled resonance widths $\widetilde{\Gamma}$ vs the interaction strength $\widetilde{\chi}$ for three representative coupling ratios: (a) $\Lambda = 1$, (b) $\Lambda = 0.5$, and (c) $\Lambda = 0.4$. Circles ($\circ$) and diamonds ($\diamond$) correspond to $k = 1$ and 0.1, respectively. In this particular example we consider $N = 10$. The solid lines are drawn for the eye and show the flow of resonance widths as $\widetilde{\chi}$ is changing. The stars ($\star$) indicate the predicted asymptotic values of the resonance widths [see Eqs. (6) and (7)]. The dashed "blue" line is the "classical" result $\Gamma_{\text{cl}}^{\pm}$.

$$\mathcal{E}_n = N\gamma\left(-\frac{i}{2} + \left(1 - 2\frac{n}{N}\right)\sqrt{\Lambda^2 - \frac{1}{4}}\right). \quad (6)$$

From this expression one can see that for $\Lambda \geq 1/2$ the resonance widths are all degenerate and equal to $N\gamma$ [see Figs. 1(a) and 1(b)]. Instead, for $\Lambda < 1/2$ the eigenvalues $\mathcal{E}_n$ are imaginary and we do not have any degeneracies for $\chi = 0$ [see Fig. 1(c)]. We have checked that whenever the widths show degeneracy the corresponding positions of resonances E_n are not degenerate, exhibiting a "dual" behavior as far as bifurcation points are concerned.

In the opposite limit of $\chi \gg 1$ one can neglect the intersite hopping term and, thus, the Hamiltonian (4) becomes diagonal leading to

$$\mathcal{E}_n = N\gamma\left[\frac{\chi}{2N\gamma}[n^2 + (N-n)^2 - N] - i\left(1 - \frac{n}{N}\right)\right]. \quad (7)$$

Therefore, we obtain N equidistant resonance widths $\Gamma_n = 2\gamma(N-n)$ corresponding to n particles being trapped on the first site (which resembles the resonance trapping phenomena known for the non interacting particles [26]). Naively
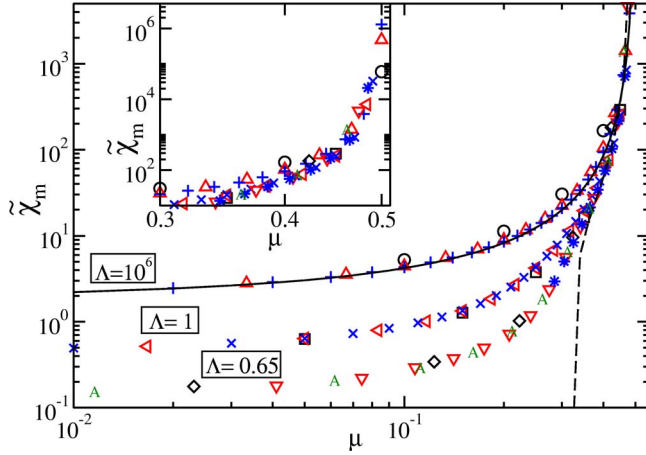
FIG. 2. (Color online) The bifurcation points $\widetilde{\chi}_m$ plotted against the scaled index μ for representative values of the dimensionless ratio $\Lambda = 0.65, 1, 10^6$. The symbols correspond to different boson numbers N and different hopping amplitudes k: $N=10$, $k=1$ (black), $N=30$, $k=10$ (red), and $N=50$ $k=20$ (blue). The symbol A corresponds to $N=20$, $k=0.1$. The solid line indicates the large N limit of the case $\Lambda = 10^6$, while the dashed line corresponds to the value $\Lambda = 0.5$ and a system size of $N=50$. In the inset we show a magnification of the main figure.

one could think that the initial degeneracy of the resonance widths for $\Lambda \geq 1/2$ can be lifted completely by arbitrary small interaction χ and the resonance widths flow continuously to their limiting values by increasing χ. Below we will see that surprisingly enough this is not the case and the degeneracy is reduced each time by 2 at $N/2$ discrete points.

In Fig. 1 we report the resonance widths for three representative values of the coupling ratio $\Lambda = 1$, 0.5, and 0.4, as a function of the interaction strength. Our numerical data are rescaled according to Eq. (1). The points corresponding to the same value of Λ (but different values of k) fall onto the same smooth curve. In the same figure we report the asymptotic values given by Eqs. (6) and (7).

In order to shed some light on the emergence of the bifurcations and the scaling ansatz (1) we adopt a semiclassical point of view for Hamiltonian (4), justified in the limit of $N \gg 1$. The corresponding classical eigenvalue problem reads

$$\mathcal{E}a_1 = \chi|a_1|^2 a_1 - ka_2,$$

$$\mathcal{E}a_2 = \chi|a_2|^2 a_2 - ka_1 - i\gamma a_2, \qquad (8)$$

which can be solved exactly. We find that for $\widetilde{\chi} < \widetilde{\chi}_{cr} = \sqrt{4 - \Lambda^{-2}}$ there are two "trivial" solutions with constant (χ-independent) value of $\Gamma = N\gamma \rightarrow \widetilde{\Gamma} = 1$ corresponding to the particles distributed equally between the two sites $|a_1|^2 = |a_2|^2 = N/2$. For $\widetilde{\chi} > \widetilde{\chi}_{cr}$ two new nontrivial solutions appear with $\Gamma_{cl}^{\pm} = \gamma N[1 \pm \sqrt{1 - 4/(\widetilde{\chi}^2 + \Lambda^{-2})}]$ corresponding to the nonequal occupations $|a_1^{\pm}|^2 = \frac{N}{2}[1 \mp \sqrt{1 - 4/(\widetilde{\chi}^2 + \Lambda^{-2})}]$. The classical results are presented also in Fig. 1 (see dashed lines). This pitchfork bifurcation is the classical analog of the quantum bifurcations discussed above.
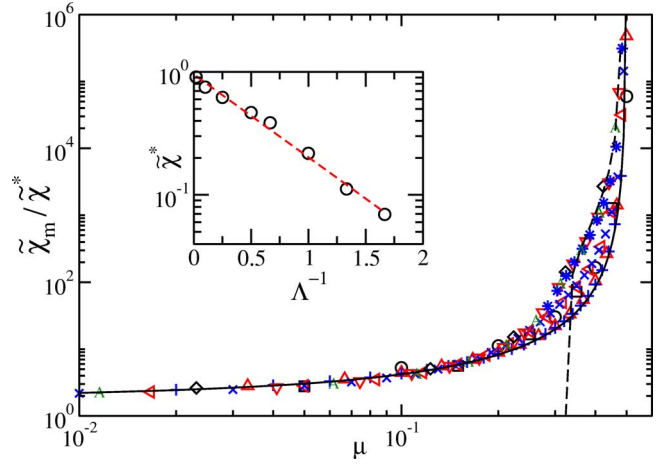

FIG. 3. (Color online) The rescaled bifurcation points $\widetilde{\chi}_m/\widetilde{\chi}^*$ for three values of $\Lambda = 0.65, 1, 10^6$. The symbols correspond to different boson numbers N and different hopping amplitudes k (see Fig. 2). The solid line indicates the large N limit of the case $\Lambda = 10^6$. Inset: the extracted scaling parameter $\widetilde{\chi}^*$ as a function of the dimensionless ratio Λ^{-1}.

We see further that for $\Lambda \geq 0.5$ resonances are initially degenerate, as is predicted by Eq. (6). As $\widetilde{\chi}$ increases this degeneracy is lifted by consequent bifurcations. Contrary, for $\Lambda \leq 0.5$ we do not observe any initial degeneracy. We note that in the regime $\Lambda < 0.5$ the instantaneous approximation is questionable since the hopping time $\tau_k \sim 1/k$ is large in comparison with the characteristic decay time $\tau_{\gamma} \sim 1/\gamma$. Therefore, in the rest of the paper we will concentrate in the opposite case $\Lambda > 0.5$ and analyze the sequences of bifurcation points $\widetilde{\chi}_m$ which we have extracted from our numerical simulations. They were identified as the points after which two degenerate resonance widths $\widetilde{\Gamma}$ differ by more than C/N, where we used $C=0.01$. In Fig. 2 we report our findings by making use of the scaling proposed in Eq. (2). An excellent agreement is evident. We have checked that our results remain qualitatively the same if we apply other similar criteria. A side remark is that the resonance positions E_n (not shown) bifurcate at the same points $\widetilde{\chi}_m$.

Now we focus on the dependence of the scaling function f_Λ on the parameter Λ. Our study has revealed the existence of a sort of transition separating two regimes characterized by different scaling properties. Namely, we found that at large μ values (i.e., large $\widetilde{\chi}$) the various Λ curves fall nicely one on top of another, even for $\Lambda = \Lambda^*$, as clearly demonstrated in the inset of Fig. 2. From our data we were able to estimate that this scaling of the upper part of the spectrum holds for $\mu \gtrsim 0.35$. Notice that in the limit of $N \rightarrow \infty$ at the fixed ratio m/N the scaling parameter $\mu \approx m/N$—i.e., is independent of Λ. In other words the bifurcations with large m values take place between states that are not affected by the intersite coupling k and the coupling to continuum γ. Indeed these states correspond to almost equidistributed number of bosons between the two traps.

On the other hand, for $\mu \lesssim 0.3$ we see that all curves, corresponding to different values of Λ, have the same functional form, albeit being shifted downwards with respect to each other (Fig. 2). The curves $\widetilde{\chi}$ do coincide, however, when

rescaling the bifurcation spectra as $\tilde{\chi}_m/\tilde{\chi}^*$ where $\tilde{\chi}^*$ is a scaling parameter (Fig. 3, main part). We find that the scaling parameter $\tilde{\chi}^*$ depends only on Λ (Fig. 3, inset) resulting in a universal one-parameter scaling for the lower part of bifurcation points according to Eq. (3). The best fitting indicates that $\tilde{\chi}^*(\Lambda) \approx \exp(-1.55\Lambda)$. We note that the scaling region becomes increasingly small as $\Lambda \to \Lambda^*$ and breaks down totally at $\Lambda = \Lambda^*$. This is the limit where the resonance widths do not show any degeneracy for $\chi=0$.

In conclusion we have studied the dependence of resonance widths of an open dimer BHH system on the strength of the on-site interaction and found a rich bifurcation behavior. Our results have immediate implications in the dynamics of an open dimer. Specifically, we expect that the decay of the bosons is not given by a simple exponential as suggested by the standard rate equation $\dot{N}=-\Gamma N$ with $\Gamma \sim \gamma$ being a constant. Instead, our analysis indicates a more complicated decay since now Γ depends on the remaining particles inside the trap [see Eq. (1) and Fig. 1], and thus one has to solve a nonlinear rate equation. The analysis of dynamics of an open BHH system is beyond the scope of the current publication and will be the subject of a separate paper.

[1] *Trends in Quantum Chaotic Scattering*, edited by Y. V. Fyodorov, T. Kottos, and H.-J. Stöckmann, J. Phys. A **38**, 10761 (2005).
[2] C. W. J. Beenakker, Rev. Mod. Phys. **69**, 731 (1997).
[3] L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, Cambridge, England, 1995).
[4] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[5] C. Mahaux and H. A Weidenmüller, *Shell Model Approach in Nuclear Reactions* (North-Holland, Amsterdam, 1969); I. Rotter, Rep. Prog. Phys. **54**, 635 (1991); J. J. M. Verbaarschot, H. A. Weidenmüller, and M. R. Zirnbauer, Phys. Rep. **129**, 367 (1985); F. Dittes, *ibid.* **339**, 215 (2000).
[6] M. H. Nayfeh *et al.*, *Atomic Spectra and Collisions in External Fields* (Plenum, New York, 1989), Vol. 2.
[7] I. Bloch, T. W. Hänsch, and T. Esslinger, Phys. Rev. Lett. **82**, 3008 (1998).
[8] T. L. Gustavson *et al.*, Phys. Rev. Lett. **88**, 020401 (2001).
[9] W. Hänsel, J. Reichel, P. Hommelhoff, and T. W. Hänsch, Phys. Rev. Lett. **86**, 608 (2001).
[10] R. Folman *et al.*, Phys. Rev. Lett. **84**, 4749 (2000).
[11] J. Schmiedmayer, R. Folman, and T. Calarco, J. Mod. Opt. **49**, 1375 (2002).
[12] T. Paul, K. Richter, and P. Schlagheck, Phys. Rev. Lett. **94**, 020404 (2005).
[13] N. Moiseyev and L. S. Cederbaum, e-print cond-mat/0406189.
[14] N. Moiseyev, L. D. Carr, B. A. Malomed, and Y. B. Band, J. Phys. B **37**, L193 (2004).
[15] P. Schlagheck and T. Paul, e-print cond-mat/0402089.
[16] T. Kottos and M. Weiss, Phys. Rev. Lett. **93**, 190604 (2004).
[17] R. Franzosi, V. Penna, and R. Zecchina, Int. J. Mod. Phys. B **14**, 943 (2000); R. Franzosi and V. Penna, Phys. Rev. A **63**, 043609 (2001).
[18] L. Bernstein, J. Eilbeck, and A. Scott, Nonlinearity **3**, 293 (1990); S. Aubry *et al.*, Phys. Rev. Lett. **76**, 1607 (1996).
[19] G. Kalosakas, A. R. Bishop, and V. M. Kenkre, Phys. Rev. A **68**, 023602 (2003); G. Kalosakas and A. R. Bishop, *ibid.* **65**, 043616 (2002); G. J. Milburn *et al.*, *ibid.* **55**, 4318 (1997).
[20] M. Albiez *et al.*, Phys. Rev. Lett. **95**, 010402 (2005).
[21] I. Barvik, B. Esser, and H. Schanz, Phys. Rev. B **52**, 9377 (1995); V. Capek and V. Szöcs, Phys. Status Solidi B **125**, 137 (1984); D. Gulen and S. Baskal, J. Phys.: Condens. Matter **5**, 899 (1993).
[22] For odd numbers of bosons, there are $(N+1)/2$ bifurcation points.
[23] We can derive Eq. (4) starting from the classical Hamiltonian $\mathcal{H}=\frac{x}{2}[|a_1|^4+|a_2|^4]-k(a_1^*a_2+a_1a_2^*)-i\gamma a_2^*a_2$, where a_i are complex amplitudes, and then apply second quantization. Here, constant terms due to symmetrization are neglected. For $\gamma=0$ this leads to the standard discrete nonlinear Schrödinger (DNLS) equation while for $\gamma \neq 0$ it leads to the DNLS equation with a sink [21].
[24] S. Kohler and F. Sols, Phys. Rev. Lett. **89**, 060403 (2002).
[25] M. J. Steel and D. F. Walls, Phys. Rev. A **56**, 3832 (1997); J. Ruostekoski *et al.*, *ibid.* **57**, 511 (1998).
[26] V. V. Sokolov and V. G. Zelevinsky, Ann. Phys. (N.Y.) **216**, 323 (1992); D. V. Savin, V. V. Sokolov, and H.-J. Sommers, Phys. Rev. E **67**, 026215 (2003).
[27] G. P. Tsironis and V. M. Kenkre, Phys. Lett. A **127**, 209 (1988); V. M. Kenkre and G. P. Tsironis, Phys. Rev. B **35**, 1473 (1987); V. M. Kenkre and D. K. Campbell, *ibid.* **34**, R4959 (1986); G. Kalosakas and A. R. Bishop, Phys. Rev. A **65**, 043616 (2002); J. C. Eilbeck, P. S. Lomdahl, and A. C. Scott, Physica D **16**, 318 (1985).