Three-Dimensional Solitary Waves and Vortices in a Discrete Nonlinear Schrödinger Lattice

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In a benchmark dynamical-lattice model in three dimensions, the discrete nonlinear Schrödinger equation, we find discrete vortex solitons with various values of the topological charge S. Stability regions for the vortices with $S = 0, 1, 3$ are investigated. The $S = 2$ vortex is unstable, spontaneously rearranging into a stable one with $S = 3$. In a two-component extension of the model, we find a novel class of stable structures, consisting of vortices in the different components, perpendicularly oriented to each other. Self-localized states of the proposed types can be observed experimentally in Bose-Einstein condensates trapped in optical lattices, and in photonic crystals built of microresonators.

Introduction. Intrinsic localized modes (ILMs), alias *discrete breathers*, in nonlinear dynamical lattices have inspired a vast array of theoretical and experimental studies. They have attracted attention due to their inherent ability to concentrate and, potentially, transport the vibrational energy in a coherent fashion (see, e.g., [1]). Settings in which these objects appear range from arrays of nonlinear-optical waveguides [2] and photonic crystals [3] to Bose-Einstein condensates (BECs) in optical-lattice (OL) potentials [4], and from various systems based on nonlinear springs [5] to Josephson-junction ladders [6] and dynamical models of the DNA double strand [7].

A benchmark model, which generically emerges in the description of dynamics in nonlinear lattices, is the discrete nonlinear Schrödinger (DNLS) equation [8]. It finds its most straightforward physical realizations in two of the above-mentioned settings, viz., arrays of optical waveguides [9,10], and networks of BEC drops trapped in OLs [4]. While the former system may be, effectively, 1- and 2-, but not 3-dimensional, the latter was experimentally created in three dimensions (3D) as well [11], which suggests a direct physical implementation of the 3D DNLS model. Another physical realization of the 3D DNLS equation may be provided by a crystal built of microresonators trapping photons [12] or polaritons [13].

In spite of the physical relevance of the NLS equation in the 3D case, very few works attempted to find localized solutions in this system, and those were actually done in the absence of OLs [14]. Only very recently, a possibility of the existence of stable 3D solitons in continuum NLS equations including OL potentials has been demonstrated [15]. A problem of fundamental interest, both in its own right and in view of the possibility of the experimental realization (principally in the BEC-OL setting), concerns the search for 3D solitons in the DNLS model proper. Especially intriguing is a possibility to construct stable ILMs with *intrinsic vorticity* (topological charge), which would be an entirely new class of ILMs in 3D.

In this work, we demonstrate that the discreteness indeed makes it possible to stabilize, in the DNLS model with attraction, not only ordinary 3D ILMs, but also vortex solitons (they are strongly unstable in the continuum limit; notice, however, that 3D vortex solitons can be stabilized in continuum models with competing nonlinearities [16]). These include not only fundamental discrete vortices, with the topological charge $S = 1$, whose stability in the 3D case may be surprising by itself, but also higher-order vortices, such as ones with $S = 3$ (in the above-mentioned 3D continuum models with competing nonlinearities, stable higher-order vortices have not yet been found). We also extend the considerations to multi-component DNLS models, that allow for the existence and stability of still more challenging configurations. In particular, we introduce a novel type of a compound vortex, consisting of two vortices with the same value of S in the two components, whose orientations are *perpendicular* to each other. Such solutions are stable too, in certain parametric intervals.

The Model. The DNLS equation on the cubic lattice with a coupling constant C is [8]

$$i\frac{d}{dt}\phi_{l,m,n} + C\Delta_2\phi_{l,m,n} + |\phi_{l,m,n}|^2\,\phi_{l,m,n} = 0, \qquad (1)$$

with $\Delta_2\phi_{l,m,n} \equiv \phi_{l+1,m,n} + \phi_{l,m+1,n} + \phi_{l,m,n+1} + \phi_{l-1,m,n} + \phi_{l,m-1,n-1} + \phi_{l,m,n-1} - 6\phi_{l,m,n}$. We seek for ILM solutions $\phi_{l,m,n} = \exp(i\Lambda t)u_{l,m,n}$, where Λ is the frequency (chemical potential in the BEC context) and the stationary eigenfunctions $u_{l,m,n}$ obey the equation

$$\Lambda u_{l,m,n} = C\Delta_2 u_{l,m,n} + |u_{l,m,n}|^2\,u_{l,m,n}. \qquad (2)$$

Due to the invariance of Eq. (1) against the scaling transformation, $t \to t/U^2$, $C \to CU^2$, and $u \to u/U$, with an arbitrary constant U, one can either fix the coupling constant, as $C \equiv C_0$, and vary Λ, with the objective to explore a full family of solutions of a certain type, or, alternatively, fix $\Lambda \equiv \Lambda_0$, and follow the variation of C. The actual control parameter, that is invariant against the scaling, is C/Λ.

Solutions to Eq. (2) (generally, complex ones) are obtained by means of a Newton method. To test their stability, perturbed solutions are used in the form [17]

$$\phi_{l,m,n} = e^{i\Lambda t}\left[u_{l,m,n} + \epsilon\left(a_{l,m,n}e^{\lambda t} + b_{l,m,n}e^{\lambda^* t}\right)\right], \quad (3)$$

where ϵ is an infinitesimal amplitude of the perturbation, and λ is its (generally, complex) eigenfrequency. The substitution of Eq. (3) into Eq. (1) gives rise to linearized equations for the perturbation eigenmodes,

$$i\lambda\begin{pmatrix} a_k \\ b_k^* \end{pmatrix} = \begin{pmatrix} \partial F_k/\partial u_j & \partial F_k/\partial u_j^* \\ -\partial F_k^*/\partial u_j & -\partial F_k^*/\partial u_j^* \end{pmatrix}\begin{pmatrix} a_k \\ b_k^* \end{pmatrix},$$

where $F_k \equiv -C(u_{k+1} + u_{k-1} + u_{k+N} + u_{k-N} + u_{k+N^2} + u_{k-N^2} - 6u_k) + \Lambda u_k - |u_k|^2 u_k$, and the string index, k, is defined so that $(l,m,n) \mapsto k \equiv l + (m-1)N + (n-1)N^2$. Dirichlet boundary conditions were imposed.

According to the scale invariance discussed above, we examine solutions of Eq. (2) by fixing the frequency, $\Lambda = 2$, and varying the coupling C (in the BEC context, this means fixing the chemical potential, and varying the OL strength, as is experimentally feasible). The solutions with different values of the topological charge S (here, it ranges between 0 and 3) are generated by an iterative scheme with an initial ansatz motivated by 3D vortices in the continuum limit [16],

$$u_{l,m,n}^{(\mathrm{init})} = A[(l-l_0) + i(m-m_0)]^S \exp\left(-|n-n_0|\right) \quad (4)$$

$$\times \mathrm{sech}\left(\eta\sqrt{(l-l_0)^2 + (m-m_0)^2}\right), \quad (5)$$

where (l_0, m_0, n_0) is the location of the vortex' center, and η is a scale parameter. The Newton algorithm was then iterated until it converged to 1 part in 10^7. Our results are typically shown for $9\times9\times9$ and $11\times11\times11$ site lattices, but larger ones were also investigated.

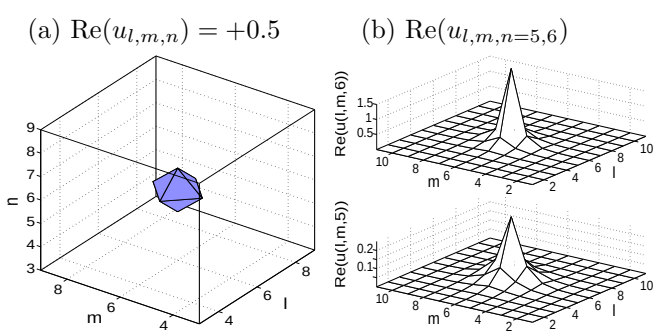

FIG. 1. The ILM with $S = 0$ is shown for $C = 1$. The left panel shows the 3D contour plot $\mathrm{Re}(u_{l,m,n}) = 0.5$. The right panels show 2D cross sections of the solution through $n = 6$ (top) and $n = 5$ (bottom) for the $11\times11\times11$ DNLS lattice.

Results. Basic results for the solutions with different topological charges can be summarized as follows. Ordinary ILMs with $S = 0$ are stable below a critical value $C_{\mathrm{cr}}^{(0)} \approx 2$ of the coupling constant, as they are strongly unstable (against collapse) in the continuum limit of $C \to \infty$. An example of a stable ordinary soliton is shown in Fig. 1. As ILMs with $S = 0$ have the largest stability interval, $C < C_{\mathrm{cr}}^{(0)}$, as compared to topologically charged ones (see below), they can only be destroyed if unstable, rather than being transformed into ILMs of other types.

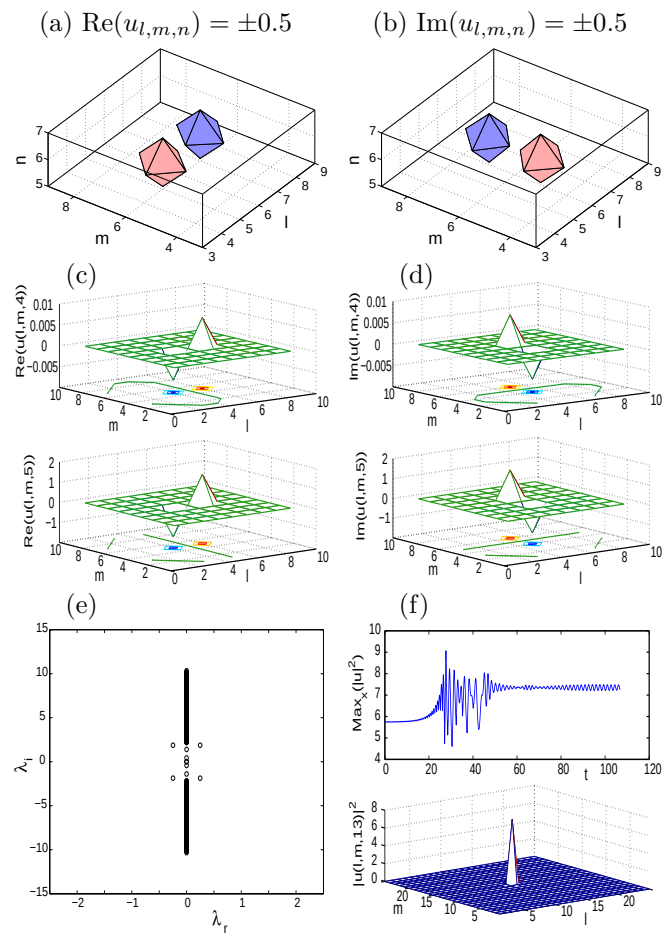

FIG. 2. The top panels show level contours at $\mathrm{Re}(u_{l,m,n}) = \pm0.5$ (left) and $\mathrm{Im}(u_{l,m,n}) = \pm0.5$ (right) for the 3D vortex ILM with $S = 1$. Red (color version) / light-gray (black-and-white) and blue/dark-gray surfaces pertain to the levels with -0.5 and $+0.5$ values, respectively. Cross sections of the vortex are shown in four middle panels, (c) and (d). The bottom row displays the development of instability of the vortex for $C = 0.7$, through the time evolution of its amplitude, and a 2D cut of the profile at $t = 100$ [(f) top and bottom, respectively]. The unstable vortex transforms itself into an ordinary ILM with $S = 0$. The left bottom panel (e) shows the spectral plane (λ_r, λ_i) of the linear stability eigenvalues for the same unstable vortex.

3D vortices with $S = 1$ have also been found. They are stable (see Fig. 2) below a critical value $C_{\mathrm{cr}}^{(1)} \approx 0.65$ (similarly to their 2D counterparts [18]). At the instability threshold, a quartet of complex eigenvalues emerges

from collision of two imaginary eigenvalue pairs (for details, see, e.g., Refs. [18,19]). Numerically simulated development of the instability is displayed in Fig. 2, for a typical case with $C = 0.7 > C_{\rm cr}^{(1)}$. The perturbations destroy the vortex structure and, as a result, an ordinary ($S = 0$) ILM emerges; obviously, the change of the topological charge is possible in the lattice, in which the angular momentum is not a dynamical invariant.

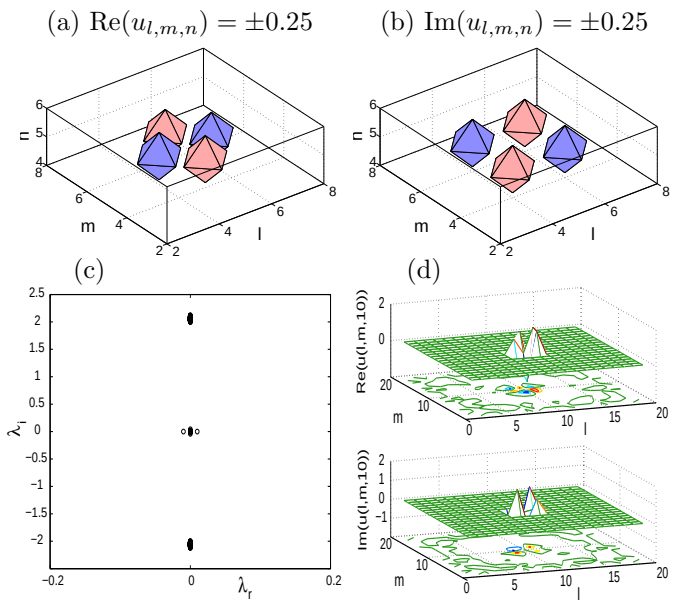

FIG. 3. The ILM vortex with $S = 2$ for $C = 0.01$. Top panels have the same meaning as the top panels in Fig. 2. The bottom left panel (c) displays the linear stability eigenvalues, while (d) shows the result of long evolution of this unstable vortex. The eventual state, shown through its 2D cross-sections at $t = 1000$, is a vortex with $S = 3$ (see Fig. 4), which is *stable* for this value of C.

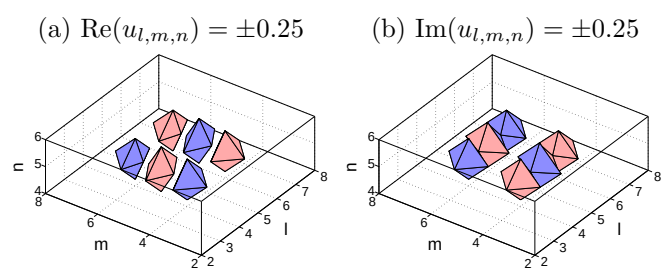

FIG. 4. Stable stationary vortex ILMs with $S = 3$ for $C = 0.01$. Panels have same meaning as top panels in Fig. 2.

An example of a vortex with topological charge $S = 2$ is shown in Fig. 3 for $C = 0.01$. Similar to its 2D counterpart [18], this complex solution is unstable through a real eigenvalue pair at all values of C (notice, however, that purely real *stable* solutions to the 2D DNLS equation, that may be identified as *quasi-vortices* similar to the solitons with $S = 2$, have been very recently found [19]; counterparts of such solutions exist in the 3D case as well). What is more interesting, however, is that this unstable ILM with $S = 2$ reshapes itself *not* into the one with $S = 0$ or $S = 1$, but rather towards a stable vortex with $S = 3$, as seen in Fig. 3. The stabilization of the 3D vortex ILM through spontaneous *increase* of S is a striking result (again, feasible only in dynamical lattices). In Fig. 4 we show the stable $S = 3$ discrete vortex for the same case, $C = 0.01$ (stable higher-order vortex ILMs were very recently found in the 2D DNLS model too [19]). The instability of the vortex with $S = 2$ vs. the stability of the vortex with $S = 3$ may be understood, in loose terms (in the 2D case as well) in terms of the lattice-induced Peierls-Nabarro (PN) potential acting on the soliton. Indeed, it is the PN potential which may stabilize a soliton which is otherwise strongly unstable. It is seen from Figs. 3 and 4 that the PN potential induced by the cubic lattice is, obviously, a much stronger factor for the soliton with $S = 3$ than with $S = 2$, due to the symmetry difference between the former one and the lattice (i.e., the "skeleton" of the vortex lies at angles of $2\pi/3$ as opposed to the $\pi/2$ of the underlying cubic lattice).

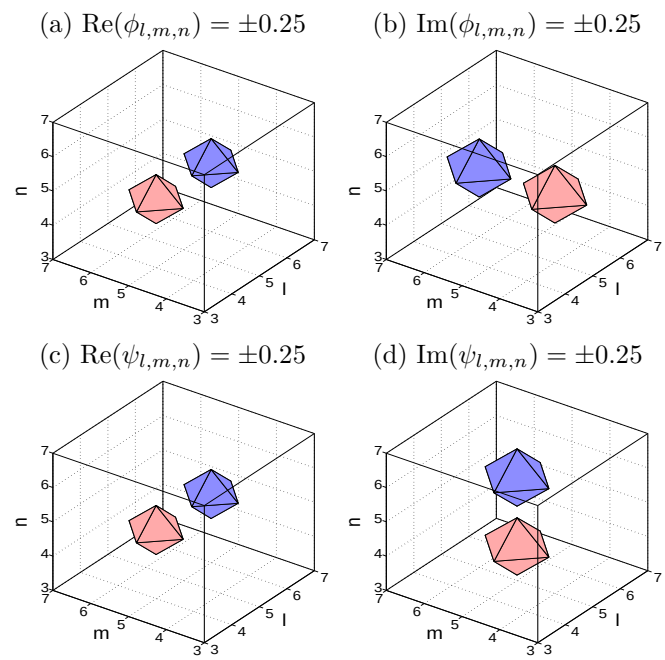

FIG. 5. A complex of two orthogonal vortices with $S = 1$ in the two-component system is shown for $C = 0.01$. The top and bottom panels correspond to the two components, and they have the same meaning as the top panels in Fig. 2.

Another striking feature, unique to the 3D case, is a possibility of the existence of vortex complexes in a multi-component system, with the vortices in different (up to three) components *orthogonal* to each other. We consider, in particular, two coupled DNLS equations,

$$\begin{aligned} \left[i\tfrac{d}{dt} + C\Delta_2 + \left(|\phi_{l,m,n}|^2 + \beta|\psi_{l,m,n}|^2\right)\right]\phi_{l,m,n} &= 0 \\ \left[i\tfrac{d}{dt} + C\Delta_2 + \left(|\psi_{l,m,n}|^2 + \beta|\phi_{l,m,n}|^2\right)\right]\psi_{l,m,n} &= 0, \end{aligned} \tag{6}$$

which describe an array of BEC droplets composed of a mixture of two different species [20]. In the case of the model based on the photon or polariton field trapped in the lattice of microresonators, ϕ and ψ refer to two different polarizations or distinct cavity modes. In Eqs. (6), β is the relative, intra-species interaction strength.

We examine a complex of two orthogonal vortices, in which the one in the first component is directed perpendicular to the (l, m) plane, while in the second component, the vortex is orthogonal to the (l, n) plane. An example of such a *stable* complex is shown, for $\beta = 0.5$, in Fig. 5. We have found that the orthogonal complexes may be stable for $\beta < 1$ (for sufficiently weak coupling C: the solutions of Fig. 5 are stable for $C < C_{cr}^{\perp} \approx 0.025$), and are unstable for $\beta > 1$. This can be qualitatively understood in terms of the Hamiltonian of the attractive interaction between the two components, each having the characteristic "doughnut" [16] vortex-soliton shape (in the continuum limit). Indeed, one can roughly estimate the interaction energy (negative) through the volume V of the overlap between two cylinders of a radius ρ (which represent long inner holes of the doughnuts) intersecting at an angle θ, $V = (20/3)\rho^3/\sin\theta$ (the divergence at $\theta \to 0$ is limited by a finite length of the holes). As it follows from here, the interaction energy has a maximum at $\theta = \pi/2$, which corresponds, by itself, to an unstable equilibrium state of two orthogonal vortices. Actually, the equilibrium is transformed into a stable one by the pinning to the PN potential, provided that the interaction is not too strong, i.e., β is not too large.

Conclusions. The above results are a first step towards an understanding of topologically nontrivial ILMs in 3D dynamical lattices. Besides generating stable ILMs without ($S = 0$) or with ($S = 1$ and 3) topological charge, the 3D lattice gives rise to a variety of novel dynamical effects, such as the reshaping of the $S = 2$ unstable vortex into a stable one with $S = 3$. Furthermore, the 3D dynamical lattice sustains quite unusual but stable states, such as the two-component complex, with the individual vortices in the components orthogonal to each other. Studying more complex configurations in such a rich setup, and examining interactions between ILMs, are challenging problems for future work.

The 3D vortices predicted in this work can be created in an self-attractive BEC trapped in an optical lattice (OL). Relevant physical parameters are essentially the same as those at which this medium is experimentally available [4,11,20], and for which various 1D and 2D localized structures were predicted [4,15], i.e., $\gtrsim 10^4$ atoms trapped in an OL with the period ~ 1 μm and the size $\gtrsim 10 \times 10 \times 10$. The soliton-formation time is ~ 1 ms, and the experiment can be easily run on the time scale of $\gtrsim 1$ s. In principle, the same vortex solitons can be also created in a cubic lattice composed of microresonators trapping photons or polaritons.

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[1] S. Aubry, Physica **103D**, 201 (1997); S. Flach and C.R. Willis, Phys. Rep. **295**, 181 (1998); see also focus issues of Physica **119D** (1999), and Chaos **13**, 586–799 (2003).

[2] See e.g., A.A. Sukhorukov *et al.*, IEEE J. Quantum Electron. **39**, 31 (2003); U. Peschel *et al.*, J. Opt. Soc. Am. B **19**, 2637 (2002).

[3] S.F. Mingaleev and Yu.S. Kivshar, Phys. Rev. Lett. **86**, 5474 (2001).

[4] A. Trombettoni and A. Smerzi, Phys. Rev. Lett. **86**, 2353 (2001); F.Kh. Abdullaev *et al.*, Phys. Rev. **A64**, 043606 (2001); F.S. Cataliotti *et al.*, Science **293** , 843 (2001); A. Smerzi *et al.*, Phys. Rev. Lett. **89**, 170402 (2002); G.L. Alfimov *et al.*, Phys. Rev. E **66**, 046608 (2002); R. Carretero-González and K. Promislow, Phys. Rev. A **66** 033610 (2002).

[5] E.N. Pelinovsky and S.K. Shavratsky, Physica **3D**, 410 (1981).

[6] P. Binder *et al.*, Phys. Rev. Lett. **84**, 745 (2000); E. Trías *et al.*, Phys. Rev. Lett. **84**, 741 (2000).

[7] M. Peyrard and A.R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989); T. Dauxois *et al.*, Phys. Rev. E **47**, R44 (1993); T. Dauxois *et al.*, Phys. Rev. E **47**, 684 (1993); M. Peyrard *et al.*, Physica **68D**, 104 (1993); A. Campa and A. Giansanti, Phys. Rev. E **58**, 3585 (1998).

[8] P.G. Kevrekidis *et al.*, Int. J. Mod. Phys. B **15**, 2833 (2001).

[9] D.N. Christodoulides and R.I. Joseph, Opt. Lett. **13**, 794 (1988); A. Aceves *et al.*, Opt. Lett. **19**, 1186 (1994).

[10] H. Eisenberg *et al.*, Phys. Rev. Lett. **81**, 3383 (1998); R. Morandotti *et al.*, Phys. Rev. Lett. **83** , 2726 (1999); H. S. Eisenberg *et al.*, J. Opt. Soc. Am. B **19**, 2938 (2002); J. Meier *et al.*, Phys. Rev. Lett. **91**, 143907 (2003).

[11] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).

[12] J.E. Heebner and R.W. Boyd, J. Mod. Opt. **49**, 2629 (2002); P. Chak *et al.*, Opt. Lett. **28**, 1966 (2003).

[13] D.M. Whittaker and J.S. Roberts, Phys. Rev. B **62**, R16247 (2000); P.G. Savvidis and P.G. Lagoudakis, Sem. Sci. Tech. **18** , S311 (2003).

[14] S. Komineas and N. Papanicolaou, Phys. Rev. Lett. **89**, 070402 (2002); Phys. Rev. A **67**, 023615 (2003).

[15] B.B. Baizakov *et al.*, J. Phys. B **35**, 5105 (2002); B.B. Baizakov *et al.*, Europhys. Lett. **63**, 642 (2003).

[16] D. Mihalache *et al.*, Phys. Rev. Lett. **88**, 073902 (2002); D. Mihalache *et al.*, Phys. Rev. E **66**, 016613 (2002).

[17] M. Johansson and S. Aubry, Phys. Rev. E **61**, 5864 (2000).

[18] B.A. Malomed and P.G. Kevrekidis Phys. Rev. E **64**, 026601 (2001).

[19] P.G. Kevrekidis, B.A. Malomed, Z. Chen, and D.J. Frantzeskakis, *Stable Higher Charge Vortices in the Discrete Nonlinear Schrödinger Equation*, submitted to Phys. Rev. E.

[20] C.J. Myatt *et al.*, Phys. Rev. Lett. **78**, 586 (1997).