Vortex families near a spectral edge in the Gross-Pitaevskii equation with a two-dimensional periodic potential

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We examine numerically vortex families near band edges of the Bloch wave spectrum for the Gross-Pitaevskii equation with two-dimensional periodic potentials and for the discrete nonlinear Schrödinger equation. We show that besides vortex families that terminate at a small distance from the band edges via fold bifurcations, there exist vortex families that are continued all the way to the band edges.

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I. INTRODUCTION

Many physical problems in periodic media with Kerr (cubic) nonlinearity are governed by the Gross-Pitaevskii equation with a periodic potential. Examples are Bose-Einstein condensates in optical lattices [1] and photonic-crystal fibers [2]. Interest in the properties of localized states in this model has stimulated a number of mathematical works devoted to this subject [3,4].

An interesting problem that arises in this context is the possibility of bifurcations of stationary localized states from the edges of Bloch bands in the wave spectrum of a Schrödinger operator with a periodic potential. The first pioneering works in this direction were completed by Stuart and his students [5–7]. In the physics literature the asymptotic approximations of gap solitons bifurcating from band edges were developed by various authors in one dimension [8,9] and two dimensions [10–12].

In one dimension it was discovered numerically in Ref. [3] and explained analytically in Ref. [13] that while single-pulse gap solitons bifurcate continuously from band edges, double-pulse gap solitons do not bifurcate from the band edges but experience fold bifurcations at a small distance from the edges. The situation becomes even more interesting in two-dimensional space where besides gap solitons, vortex solutions are possible in periodic potentials [14–16]. However, a contradiction arises between the analytical results of Refs. [15,16], suggesting a continuous family of the fundamental vortex solutions bifurcating from the band edges, and the numerical results of Ref. [14], suggesting a fold bifurcation of vortex families at a small distance from the band edges. This contradiction will be inspected in this paper by using numerical computations.

We will show that there do exist continuous families of the fundamental vortex solutions bifurcating from band edges, according to the theory in Refs. [15,16]. Numerical approximations of these families near band edges suffer, however, from the fact that the vortex localization is too broad and hence extends beyond the chosen computational domain. As a result, a spurious fold bifurcation occurs for the fundamental vortex family before the family reaches the band edge. If the size of the computational domain is enlarged, the location of the spurious fold bifurcation moves closer to the band edge. At the same time there are other vortex families, found also in Ref. [14], which feature a true fold bifurcation at a small distance from a band edge. The fold location is independent of the size of the computational domain for these vortex families.

The paper is organized as follows. Section II introduces the two models which we inspect, namely, the Gross-Pitaevskii equation with a periodic potential and the discrete nonlinear Schrödinger equation. The connection between these models as well as the asymptotics of gap solitons near the band edges are reviewed. Section III gives numerical results for the family of fundamental vortices. Section IV illustrates fold bifurcations for families of quadrupole and dipole vortex configurations. In Sec. V we summarize our findings.

II. MODELS

The stationary Gross-Pitaevskii equation with a periodic potential in the two-dimensional space takes the form

$$-\Delta\varphi + V(x,y)\varphi - |\varphi|^2\varphi = \omega\varphi, \quad (x,y) \in \mathbb{R}^2, \tag{1}$$

where the focusing case is considered, the 2π periodic potential V in each coordinate is assumed to be bounded, and $\omega \in \mathbb{R}$ is taken in a spectral gap of the Schrödinger operator

$$L_0 := -\Delta + V.$$

For simplicity, we assume that the periodic potential V has even symmetries with respect to reflections about $x = 0$ and $y = 0$.

When ω is close to the upper edge ω_0 of a spectral gap of L_0, a slowly varying envelope approximation of localized states can be derived and rigorously justified for the focusing stationary Gross-Pitaevskii equation [15,16]. In the simplest case when ω_0 is attained by only one extremum of the band structure and the Hessian at the extremum is definite, the resulting approximation is

$$\varphi(x,y) = \varepsilon\psi(\varepsilon x,\varepsilon y)\varphi_0(x,y) + \mathcal{O}_{H^s}(\varepsilon^{2/3}), \quad \omega = \omega_0 - \varepsilon^2, \tag{2}$$

where $s > 1$ is arbitrary, φ_0 is the Bloch function at the band edge ω_0, and $\psi = \psi(X,Y)$ in slow variables $X = \varepsilon x$ and $Y = \varepsilon y$ satisfies the stationary nonlinear Schrödinger (NLS) equation. This effective NLS equation is written in the form

$$\alpha\,(\psi_{XX} + \psi_{YY}) + \beta|\psi|^2\psi = \psi, \tag{3}$$

where $\alpha > 0$ is related to the band curvature at the point ω_0 and $\beta > 0$ is related to a norm of the Bloch function φ_0. We note that if $\psi \in H^s(\mathbb{R}^2)$, then the leading-order term

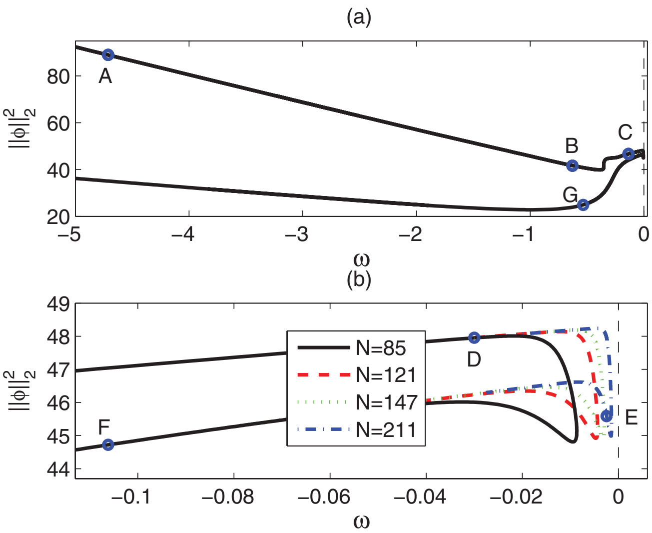

FIG. 1. (Color online) Family of vortex solutions of Eq. (7) continued from the vortex (6) via the envelope approximation (8) at $\omega = -0.03$ (point D). (a) A fixed computational domain is used with $N = 85$. (b) Detail of the vicinity of the spectral edge for a range of sizes of the computational domain.

$\varepsilon\psi(\varepsilon x,\varepsilon y)\varphi_0(x,y)$ has the order $\mathcal{O}_{H^s}(1)$ as $\varepsilon \to 0$ [16], and hence expansion (2) shows that the perturbation term is smaller than the leading-order term in the H^s norm where $H^s(\mathbb{R}^2)$ is the Sobolev space of square integrable functions on $(x,y) \in \mathbb{R}^2$ and their derivatives up to the sth order. When ω_0 is the (upper) edge of the semi-infinite gap, the error was shown to be $\mathcal{O}_{H^s}(\varepsilon)$ or $\mathcal{O}_{L^\infty}(\varepsilon^2)$ [12].

The main theorem of Refs. [15,16] states that if $\psi \in H^s(\mathbb{R}^2)$ satisfies certain reversibility symmetries such as

$$\psi(X,Y) = \pm\bar{\psi}(-X,Y) = \pm\bar{\psi}(X,-Y) \tag{4}$$

or

$$\psi(X,Y) = \pm\bar{\psi}(Y,X) = \pm\bar{\psi}(-Y,-X) \tag{5}$$

and if the linearization of the stationary NLS Eq. (3) is nondegenerate, then a localized solution of the Gross-Pitaevskii Eq. (1) with the asymptotic expansion (2) exists in $H^s(\mathbb{R}^2)$ for this ψ. In particular, the stationary NLS Eq. (3) admits the fundamental vortex of charge $m \in \mathbb{N}$ in the form

$$\psi(X,Y) = \rho(R)e^{im\theta}, \quad R = \sqrt{X^2+Y^2}, \quad \theta = \arg(X+iY), \tag{6}$$

where $\rho(R) > 0$ for all $R > 0$ satisfies a certain differential equation that follows from the stationary NLS Eq. (3). Vortex solution (6) satisfies symmetry (4), and the linearization of Eq. (3) at this ψ is nondegenerate. Hence, the conditions of the main theorem in Refs. [15,16] are validated, and there exists a unique localized solution of Eq. (1) continued from this ψ with the asymptotic expansion (2). The continuation of fundamental vortices is considered in Sec. III.

In the tight-binding limit of narrow spectral bands, several authors [17–19] rigorously justified an approximation of localized states of the stationary Gross-Pitaevskii Eq. (1) by the localized states of the stationary discrete nonlinear Schrödinger (DNLS) equation

$$-(\Delta_{\rm disc}\phi)_{m,n} - |\phi_{m,n}|^2\phi_{m,n} = \omega\phi_{m,n}, \quad (m,n) \in \mathbb{Z}^2, \tag{7}$$

where

$$(\Delta_{\rm disc}\phi)_{m,n} = \phi_{m+1,n} + \phi_{m,n+1} + \phi_{m-1,n} + \phi_{m,n-1} - 4\phi_{m,n}$$

and $\omega \notin \sigma(-\Delta_{\rm disc}) = [0,8]$. The DNLS equation simplifies numerical approximations compared with the continuous Gross-Pitaevskii equation but does not change the properties of the localized states. In particular, bifurcations of localized states are possible from the band edge $\omega = 0$ in the focusing case. Moreover, the same method of asymptotic multiscale expansions can be adopted to the DNLS Eq. (7) with the expansion

$$\phi_{m,n} = \varepsilon\psi(\varepsilon m,\varepsilon n) + o_{l^2}(1), \quad \omega = -\varepsilon^2, \tag{8}$$

where ψ satisfies the same stationary NLS Eq. (3). A rigorous justification of the continuous NLS equation as an asymptotic model for ground states of the DNLS equation was recently developed in Refs. [20,21].

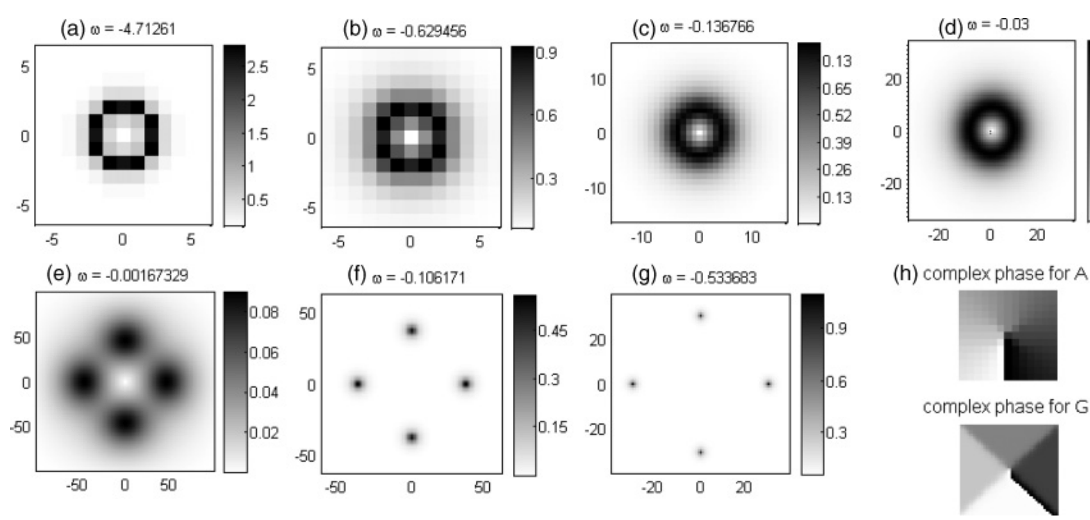

FIG. 2. (a)–(g) Modulus of the discrete vortex solutions labeled A–G in Fig. 1. (h) Plots of the complex phases for vortices A and G.

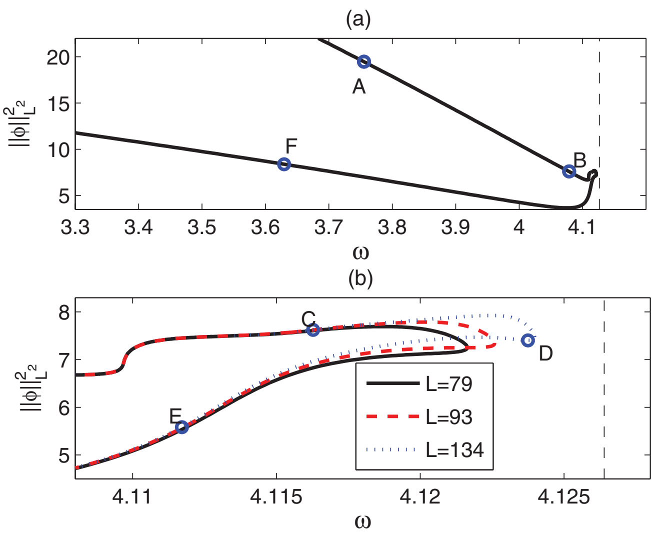

FIG. 3. (Color online) Family of vortex solutions of Eq. (1) continued from the vortex (6) via the envelope approximation (2) at $\omega \approx 4.09$ (point B). (a) A fixed computational domain is used with $L = 93$. (b) Detail of the vicinity of the spectral edge for a range of sizes of the computational domain.

III. VORTEX FAMILY CONNECTED TO THE SPECTRAL EDGE

We compute here a family of the fundamental vortices in the DNLS Eq. (7) by using the near-edge asymptotics (8) with ψ given by the continuous vortex (6). We will also compare this behavior with the one in the Gross-Pitaevskii Eq. (1).

Choosing the vortex in the form of Eq. (6) with $m = 1$, we compute the positive spatial profile ρ by the shooting method. We set $\varepsilon = \sqrt{0.03}$ so that the expansion (8) produces an initial guess for a solution ϕ of the DNLS Eq. (7) with $\omega = -0.03$ and compute ϕ via Newton's method.

Next, we continue the family in the $(\omega, \|\phi\|^2_{l^2})$ plane using the pseudo-arc-length continuation [22] in which both ϕ and ω are unknowns, combined with Newton's method. The resulting solution family is plotted in Fig. 1(a) using the computational domain $[-42,42]^2 \subset \mathbb{Z}^2$. The starting point at $\omega = -\varepsilon^2 = -0.03$ is marked as D in Fig. 1(b).

The family of vortices with charge $m = 1$ seems to fold and never reach the spectral edge, contrary to the approximation (8). In Fig. 1(b) this folding is, however, shown to be merely a numerical artifact caused by the truncation of the infinite domain $\mathbb{Z}^2$. The fold location approaches the edge $\omega = \omega_0 = 0$ as the computational domain is enlarged. The family branch containing A–D thus terminates at the edge if computed on domains of diverging size.

In the vicinity of the fold bifurcation, the solutions are inherent to the truncated domain and do not correspond to any solution of the DNLS Eq. (7) on $\mathbb{Z}^2$. The fold divides the family into two branches. Only the first branch, containing the points A, B, C, and D, is a continuation of the vortex family with the asymptotics given by Eq. (8) with ψ as the continuous vortex (6). The other branch corresponds to a different family of vortex solutions.

Figure 2 shows the solutions labeled A–G in Fig. 1. The limiting behavior for $\omega \to -\infty$ along the branch with A and B is a vortex with a square structure with sides of length five and three active sites on each side, i.e., the excited sites are at

$$(-1,-2),(0,-2),(1,-2),(-1,2),(0,2),(1,2),(-2,-1),$$
$$(-2,0),(-2,1),(2,-1),(2,0),(2,1) \in \mathbb{Z}^2.$$

Along the other branch beyond the point G in the direction of decreasing ω, the four solution peaks are further localized approaching single-site excitations as $\omega \to -\infty$. The vortices

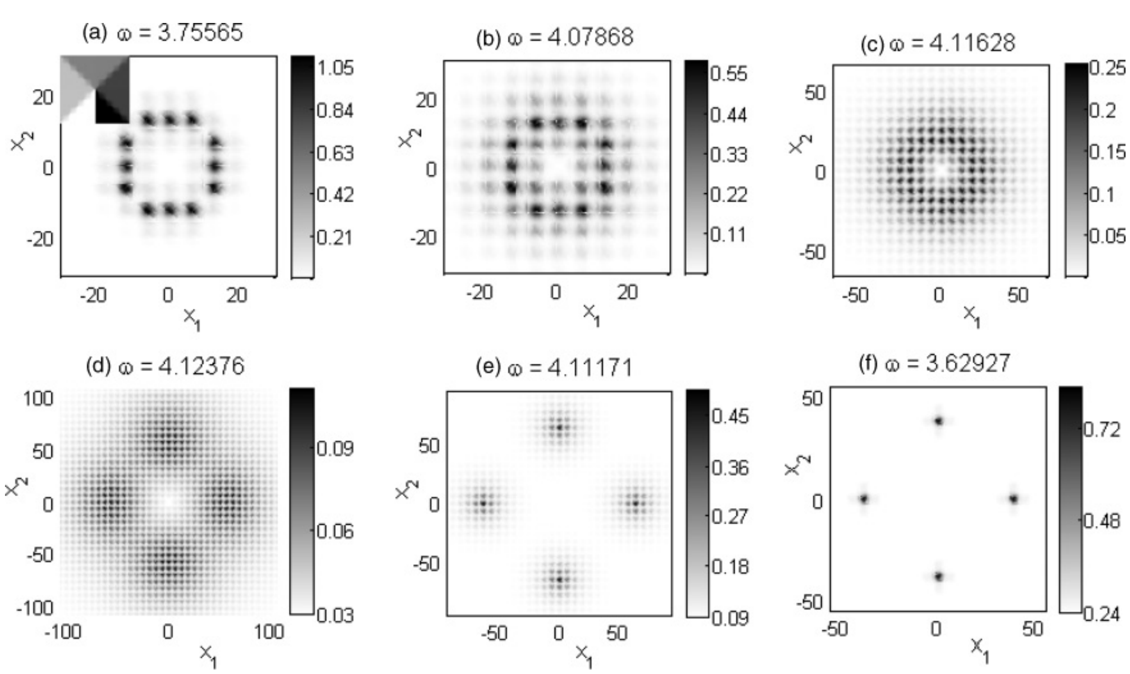

FIG. 4. Modulus of the continuous vortex solutions labeled in Fig. 3. The inset in (a) shows a qualitative plot of the complex phase.

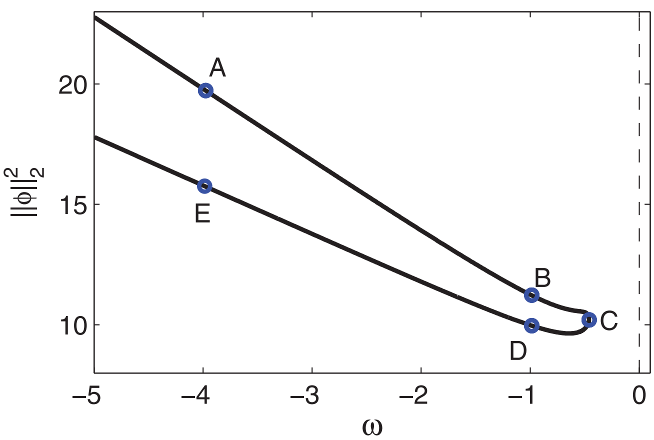

FIG. 5. (Color online) Family of discrete vortex solutions continued from a quadrupole vortex and four nearest neighbor excited sites as $\omega \to -\infty$.

keep the charge among the whole family. The complex phase for vortices A and G is plotted in Fig. 2(h).

A similar situation arises for vortex solutions of the continuous Gross-Pitaevskii Eq. (1). In Figs. 3 and 4, we present a family of vortices for

$$V(x,y) = 6\sin^2(x) + 6\sin^2(y),$$

which was the potential used in Ref. [14]. We consider the vicinity of the lowest spectral edge $\omega_0 \approx 4.1264$. The selected family is qualitatively similar to the discrete vortex family above and also terminates at the gap edge. The computational domain is $[-L/2,L/2]^2 \subset \mathbb{R}^2$, and the stationary Eq. (1) is discretized via central difference formulas of order 4.

The results of this section contradict the claim from Ref. [14] that no vortex families can be continued to the band edge of the Bloch spectrum. These results illustrate the validity of the main theorems from Refs. [15,16], which point out the possibility of such continuations for solutions satisfying reversibility symmetries (4) or (5) and the nondegeneracy conditions, e.g., for the fundamental vortex solutions.

IV. QUADRUPOLE AND DIPOLE VORTEX FAMILIES DISCONNECTED FROM THE SPECTRAL EDGE

A classical example of a vortex solution of the Gross-Pitaevskii Eq. (1) and of the DNLS Eq. (7) is the quadrupole vortex with the four nearest neighbor sites excited in a square arrangement in the asymptotics $\omega \to -\infty$, i.e., with the excited sites at

$$(-1,0),(1,0),(0,-1),(0,1) \in \mathbb{Z}^2.$$

For the Gross-Pitaevskii equation, the excited sites are understood as locations of the single wells (minima) of the periodic potential V. We obtain this family for the DNLS equation via the initial guess

$$\phi_{m,n} = 2\delta_{m,1}\delta_{n,0} + 2i\delta_{m,0}\delta_{n,1} - 2\delta_{m,-1}\delta_{n,0} - 2i\delta_{m,0}\delta_{n,-1}, \quad (m,n) \in \mathbb{Z}^2,$$

at $\omega = -1.2$ (point D in Fig. 5), where $\delta_{m,m_1}\delta_{n,n_1}$ is the Kronecker unit vector at (m_1,n_1) on $\mathbb{Z}^2$. The family is then continued, once again, via the pseudo-arc-length continuation combined with the Newton iteration.

In Figs. 5 and 6 the family curve and several solution profiles are plotted. The computation was performed on the domains $[-N,N]^2$ with $N = 10,16,20,40$, and the curves in the $(\omega,\|\phi\|_{l^2}^2)$ plane remained within the distance of $\mathcal{O}(10^{-6})$ for all these N and did not approach the edge. This family folds and does not reach the spectral edge, and all its solutions remain tightly localized. It does not, therefore,

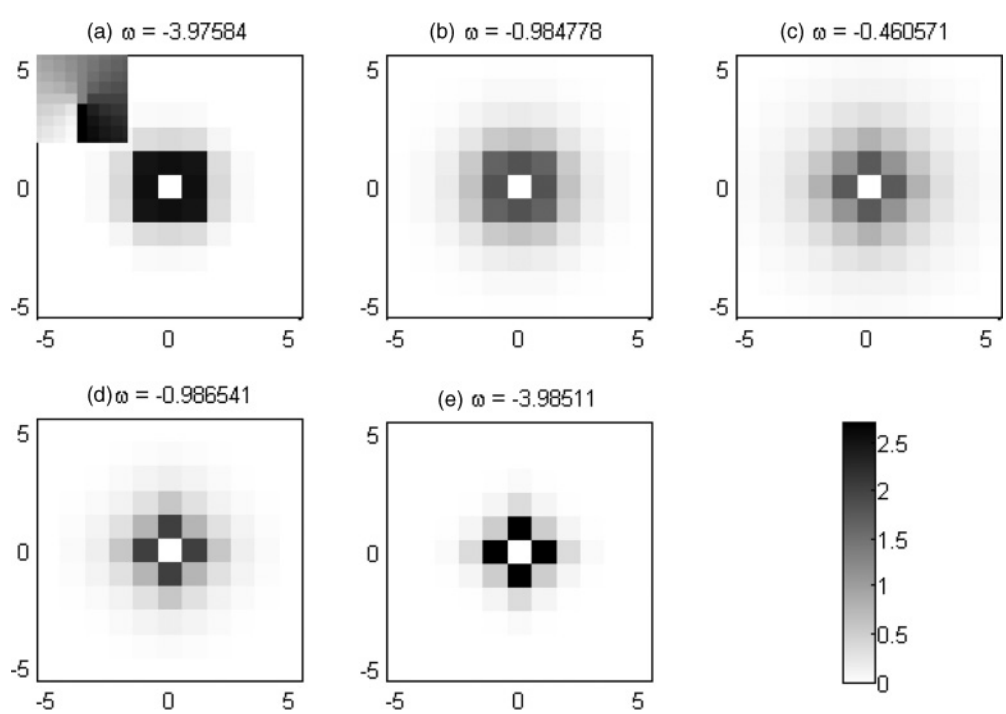

FIG. 6. Modulus of the discrete quadrupole vortex solutions labeled in Fig. 5. The inset in (a) shows a qualitative plot of the complex phase.

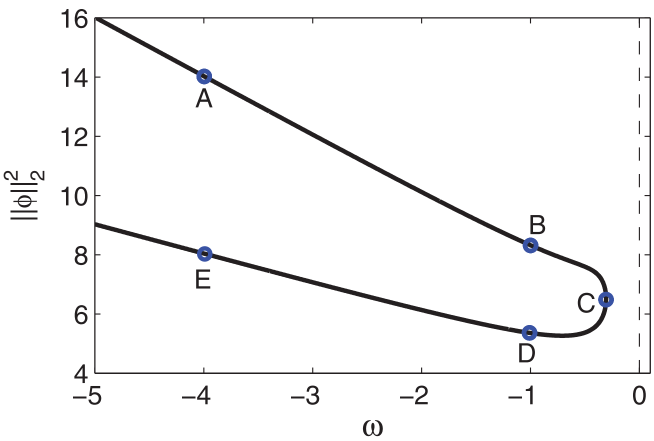

FIG. 7. (Color online) Family of discrete vortex solutions continued from a dipole vortex with two nearest neighbor excited sites as $\omega \to -\infty$.

contain a slowly varying solution near the band edge, which could be approximated via the envelope approximation (8). Qualitatively, this family corresponds to the family *a–d* in Fig. 1(a) of Ref. [14]. The branch past the fold, i.e., the branch with A and B, has as the asymptotic profile for $\omega \to -\infty$ a square vortex with excited sites at

$$(-1,-1),(-1,0),(-1,1),(0,1),(1,1),(1,0),$$
$$(1,-1),(0,-1) \in \mathbb{Z}^2.$$

We also consider a family of real dipole solutions ϕ which are odd in the n index and satisfy $\phi_{m,0} = 0$ for all $m \in \mathbb{Z}$. It is constructed via the "handmade" initial guess

$$\phi_{m,n} = 1.5\delta_{m,0}\delta_{n,1} - 1.5\delta_{m,0}\delta_{n,-1}, \quad (m,n) \in \mathbb{Z}^2,$$

at $\omega = -1.2$ (point D in Fig. 7). The family is plotted in Figs. 7 and 8. The computation was performed on the domains $[-N,N]^2 \in \mathbb{Z}^2$ with $N = 10,15,20,40$, and the curves in the $(\omega,\|\phi\|_{l^2}^2)$ plane remained within the distance of $\mathcal{O}(10^{-5})$ from each other for all these N and did not approach the edge. This family contains again only tightly localized solitons and does not continue to the spectral edge either. Along the branch with points E and D, the asymptotic profile for $\omega \to -\infty$ is the dipole with the excited sites $(0,-1)$ and $(0,1)$. Along the other branch, the asymptotic profile is twice as broad with the excited sites at

$$(0,-2),(0,-1),(0,1),(0,2) \in \mathbb{Z}^2.$$

The results of this section confirm the previous numerical results from Ref. [14] in which all quadrupole vortex families have a fold bifurcation at a small distance from the band edge of the Bloch spectrum. Solutions throughout our quadrupole and dipole families remain tightly localized so that they are not compatible with the slowly varying approximation (8). It is, however, possible that there exist other solution families, which have a dipole or quadrupole asymptotic form as $\omega \to -\infty$ and which bifurcate from the spectral edge. The bifurcation would be guaranteed by the results of Refs. [15,16] if the continuous NLS Eq. (3) had dipole or quadrupole solutions, which we are not aware of.

V. CONCLUSION

We have numerically demonstrated in both the Gross-Pitaevskii equation with a two-dimensional periodic potential and the discrete nonlinear Schrödinger equation that there are families of fundamental vortices bifurcating from spectral edges of the Bloch wave spectrum. This is in agreement with the analysis in Refs. [15,16] and in contradiction with the

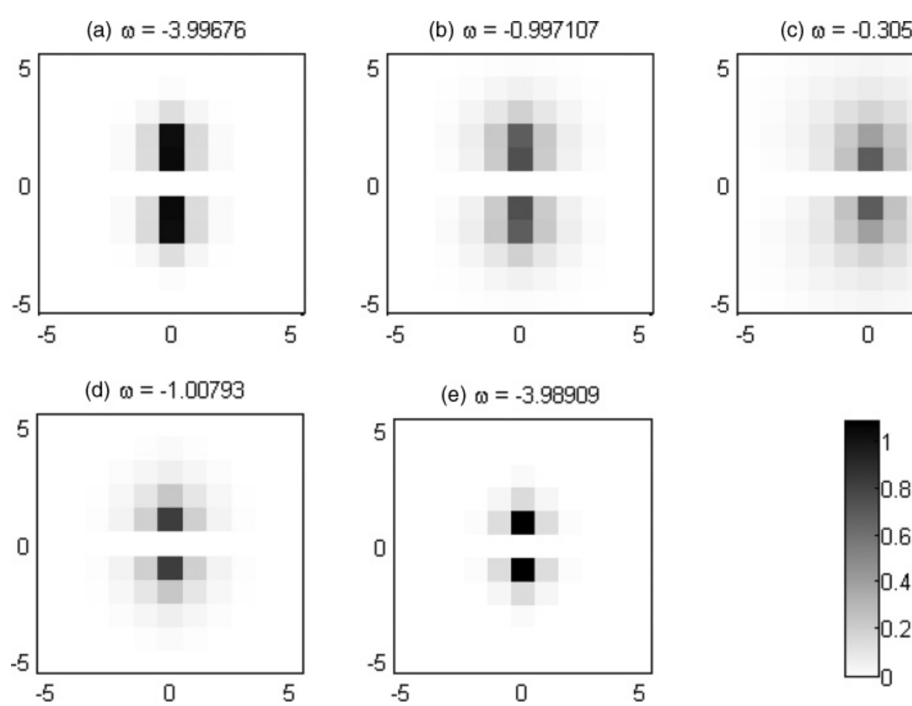

FIG. 8. Modulus of the discrete dipole vortex solutions labeled in Fig. 7.

claim in Ref. [14] that no vortex families continue to a spectral edge. Our fundamental vortex families complement the vortex families constructed in Ref. [14], which all terminate at a distance from the spectral edge via a fold bifurcation.

We have also investigated families of quadrupole and dipole vortex configurations of the DNLS equation. The selected families do terminate via fold bifurcations, which are located at a small distance from the band edge, independent of the size of the computational domain. It is an open question whether there exist other families of quadrupole and dipole vortex configurations which bifurcate from spectral edges of the Bloch wave spectrum.

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