

## Surface Bound States in the Continuum

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We introduce a novel concept of surface bound states in the continuum, i.e., surface modes embedded into the linear spectral band of a discrete lattice. We suggest an efficient method for creating such surface modes and the local bounded potential necessary to support the embedded modes. We demonstrate that the surface embedded modes are structurally stable, and the position of their eigenvalues inside the spectral band can be tuned continuously by adding weak nonlinearity.

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Soon after the emergence of quantum mechanics, von Neumann and Wigner suggested [1] that certain potentials could support spatially localized states within the continuum spectrum, i.e., bound states with energies above the potential barriers. Since 1929, when this remarkable proposal was published, the bound states in the continuum have been regarded as a mathematical curiosity, even though such potentials were suggested to occur in certain atomic and molecular systems [2,3]. Subsequent experiments with semiconductor heterostructures provided the direct observation of electronic bound states above a potential well localized by Bragg reflections [4].

In addition to the physics of electronic structures and quantum dot systems, this topic attracted a lot of attention in optics [5–7], where it was very recently shown that the optical bound states can be generated in an optical waveguide array by decoupling from the continuum by virtue of symmetry only [8].

In this Letter, we extend the pioneering concept of von Neumann and Wigner [1] into two novel directions. First, we demonstrate that the bound states can exist in systems of a semi-infinite extent as surface bound states in the continuum. We suggest and implement a novel method for creating square-integrable, discrete surface modes embedded into a linear spectrum. Such surface modes can be regarded as a novel type of localized surface Tamm-like states with energies in the continuum (i.e., “embedded Tamm modes”). Second, we study the properties of such embedded states in the presence of nonlinearity and demonstrate that the mode location inside the band can be tuned continuously by changing the mode amplitude. Importantly, our modes appear in entirely asymmetric systems and therefore, cannot be reduced by any means to the bound states in infinite systems analyzed before where the decoupling from the continuum occurs due to the symmetry conditions.

We consider a semi-infinite, one-dimensional linear lattice, in the presence of a site energy distribution  $\{\epsilon_n\}$

(Fig. 1). In optics, this could correspond to a set of weakly coupled optical waveguides [8], each of them characterized by a propagation constant  $\epsilon_n$  and centered at  $x_n = na$ . In the coupled-mode approach, we expand the electric field  $E(x, z)$  as a superposition of the fundamental modes centered at each waveguide,  $E(x, z) = \sum_n C_n(z) \phi(x - na)$ , where  $\phi(x)$  is the waveguide mode. We pose  $C_n(z) = C_n \exp(i\lambda z)$ . After inserting this into the paraxial wave equation, one obtains the stationary equations for the mode amplitudes

$$(-\lambda + \epsilon_n)C_n + V(C_{n+1} + C_{n-1}) = 0, \quad n > 1, \quad (1)$$

and the similar equation for the edge waveguide,

$$(-\lambda + \epsilon_1)C_1 + VC_2 = 0, \quad n = 1. \quad (2)$$

From these equations, we can formally express

$$\epsilon_n = \begin{cases} \lambda - V\left(\frac{C_2}{C_1}\right) & \text{if } n = 1; \\ \lambda - V\left(\frac{C_{n+1}}{C_n} + \frac{C_{n-1}}{C_n}\right) & \text{if } n > 1. \end{cases} \quad (3)$$

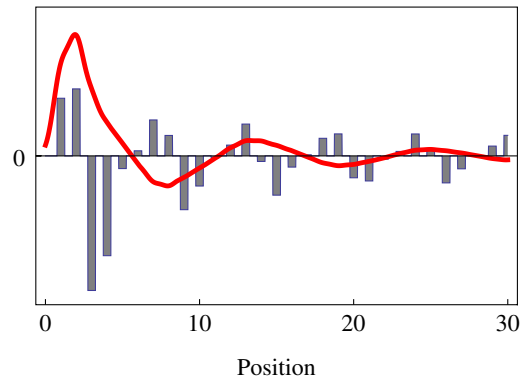


FIG. 1 (color online). Example of the site energy distribution (grey bars) and its associated surface bound state (solid curve) with energy inside the continuum spectrum.

For a homogeneous system, we take  $\epsilon_n = 0$ , and

$$C_n = \sin(kn) \quad \text{and} \quad \lambda = 2V \cos(k). \quad (4)$$

For  $\epsilon_n \neq 0$ , and in the spirit of the concept of von Neumann and Wigner [1], we look for a localized surface mode in the shape of a modulated wave of the form

$$C_n = \sin(nk)f_n \quad (5)$$

where  $f_n \rightarrow 0$  for  $n \rightarrow \infty$ , in order to realize a localized state. After inserting this ansatz into (1), we obtain

$$\epsilon_n = \begin{cases} \lambda - 2V(f_2/f_1)\cos(k) & \text{if } n = 1 \\ \lambda - V\{(f_{n+1}/f_n)[\cos(k) + \sin(k)\cot(kn)] \\ + (f_{n-1}/f_n)[\cos(k) - \sin(k)\cot(kn)]\} & \text{if } n > 1, \end{cases} \quad (6)$$

and we have  $\lim_{n \rightarrow \infty} \epsilon_n = 0$ , provided that  $\lim_{n \rightarrow \infty} (f_{n+1}/f_n) = 1$ .

Let us take

$$\frac{f_{n+1}}{f_n} = (1 - \delta_n) \quad (7)$$

where  $\delta_n < 1$ . From this, we can solve formally for  $f_n$ :

$$f_n = \prod_{m=1}^{n-1} (1 - \delta_m) \quad (8)$$

which can be rewritten as

$$f_n = \exp\left\{\sum_{m=1}^{n-1} \log(1 - \delta_m)\right\}. \quad (9)$$

In the limit  $n \rightarrow \infty$ , and using that  $\delta_m < 1$ , we can approximate this by

$$f_\infty \approx \exp\left\{-\sum_{m=1}^{\infty} \delta_m\right\} \quad (10)$$

where, we want  $f_\infty \rightarrow 0$ . This implies  $\sum_{m=1}^{\infty} \delta_m = \infty$ . A good trial function for  $\delta_n$  is

$$\delta_n = \frac{1}{\sqrt{n}} \sin^2(nk) \sin^2[(n+1)k]. \quad (11)$$

The presence of the sine terms is not accidental; we need them to counteract the presence of the two  $\cot(nk)$  terms in (6) that may otherwise lead to possible divergences. In this way, we get a smoother site energy distribution. A useful parameter to quantify the degree of localization of a state, is its participation ratio  $R$ , defined by,  $R \equiv (\sum_n |C_n|^2)^2 / \sum_n |C_n|^4$ . For localized modes,  $R \approx 1$  while for extended states  $R \approx N$ , where  $N$  is the number of sites in the lattice.

Figure 2 shows results for a lattice of  $N = 533$  sites, using the trial function (11) and  $k = 0.56$ . The mode approaches zero slowly but surely. The asymptotic decay of the envelope at large  $n$  values can be estimated, using the

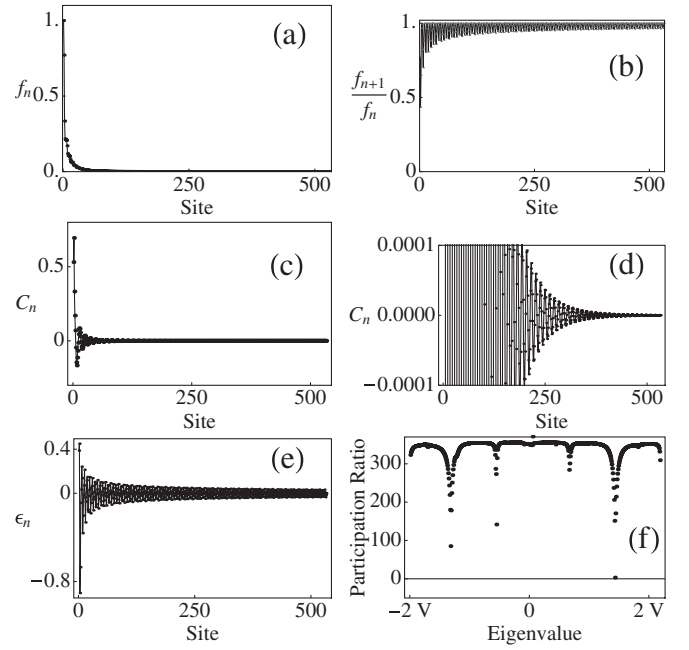


FIG. 2. (a) Discrete envelope function  $f_n$  vs  $n$ . (b) Ratio of the envelope functions at the neighboring sites. (c) Embedded mode profile. (d) Close up of the panel (c). (e) Site energy distribution and (f) participation ratio of all eigenvectors of the linear modes. ( $k = 0.56$ ,  $N = 533$ ).

Euler-Maclaurin formula, to be  $C_n \sim \sin(kn) \times \exp(-\alpha(k)\sqrt{n})$ , with  $\alpha(k) = [2 + \cos(2k)]/4$ . Figure 2 also shows the site energy distribution  $\epsilon_n$  and participation ratio  $R$  of all modes inside the band (outside the band, there are 10 “impurity” localized states), and we see that our candidate for the embedded mode (with eigenvalue  $\lambda = 1.695$ ) has the lowest of them all,  $R \approx 3$ . The next higher  $R$  value is  $\approx 85$ . Figure 3 shows the states inside the band that are closest in energy to the embedded state. The embedded state is the only state inside the band whose amplitude decreases to zero at large distance from the surface ( $n = 1$ ), while all the rest of the band states are extended.

Next, we proceed to check the structural stability of the embedded mode. That is, whether the mode is stable against perturbations caused, for instance by errors in the form of the site energy distribution (refraction index distribution in optics). This can happen during an attempt to reproduce experimentally the embedded mode. We took a lattice of 333 sites and examined two cases: First, the energy site distribution  $\{\epsilon_n\}$  is replaced with another  $\epsilon_n \rightarrow \epsilon_n + \delta_n$ , where  $\delta_n$  is a random number taken from a uniform random distribution whose width is proportional to the  $\epsilon_n$  at a given site. For instance, we took  $\delta_n \in [-0.1|\epsilon_n^{\text{old}}|, 0.1|\epsilon_n^{\text{old}}|]$ . The old and new energy site distribution look nearly the same, and as a result, the old given  $\lambda$ , just shifts a little bit. The number of states outside the band does not change and we still have an embedded mode, surrounded by extended modes, as in Fig. 3. Next, we try a

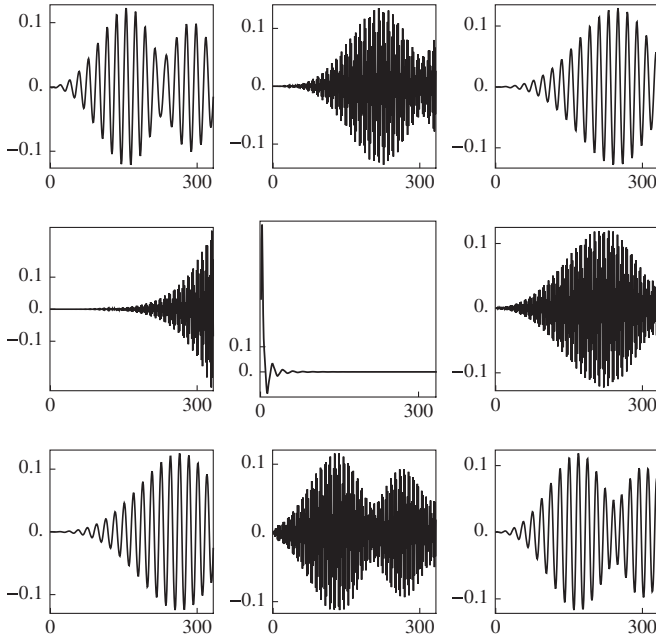


FIG. 3. States in the spectrum band that are the closest in energy to the embedded mode (middle panel) ( $N = 333$ ,  $k = 0.33$ ).

more drastic perturbation, where  $\delta_n$  is now drawn from a uniform random distribution which does not depend on site position:  $\epsilon_n^{\text{new}} = \epsilon_n^{\text{old}} + \delta_n$  where,  $\delta \in [-0.1, 0.1]$ . We see in this case that, even though the  $\epsilon_n$  becomes significantly distorted far from the boundary, the embedded state, with eigenvalue 1.892 08 survives, with a different eigenvalue 1.851 74. Whether the new eigenvalue is smaller or larger than the original one, depends on the random realization. Figure 4 shows the old and new site energy distribution, while Fig. 5 shows the new band states surrounding the new embedded mode. The spatial profiles of all of them maintain their extended nature, save for a small tendency towards localization, in agreement with Anderson localization theory. As long as the disorder is small and Anderson's localization length is much larger than the dimensions of the lattice, the localized embedded state is well defined.

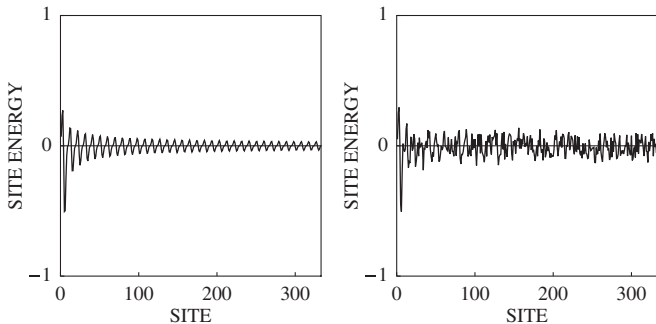


FIG. 4. Original (left) and randomly perturbed (right) site energy distribution ( $N = 333$ ,  $k = 0.33$ ).

We can then conclude that the embedded state is structurally stable against small perturbations.

Finally, we address the issue of possible tunability of the embedded state. Starting from a given embedded mode  $\lambda$ , we would like to be able to change its position inside the band, without altering the original site energy distribution. An attractive way to do this, accessible in optics, is by introducing a small amount of nonlinearity into the system. A similar approach has been explored recently for the tuning of localized modes in photonic-crystal waveguides with side-coupled symmetric defects [9].

For Kerr nonlinearity, all state eigenvalues will be shifted by the amount  $\gamma|C_n|^2$ . For extended states, the effect will be negligible, and the only state that can be affected, is the localized one. In the presence of a nonlinear response, the discrete equations (1) and (2) become:

$$(-\lambda + \epsilon_n + \gamma|C_n|^2)C_n + V(C_{n+1} + C_{n-1}) = 0, \quad n > 1, \quad (12)$$

and the equation for the edge waveguide

$$(-\lambda + \epsilon_1 + \gamma|C_1|^2)C_1 + VC_2 = 0, \quad n = 1, \quad (13)$$

where  $\gamma = 1(-1)$  denotes attractive (or repulsive) nonlinearity. At this point, it is useful to make the change of variables  $\phi_n = C_n/\sqrt{P}$ , where  $P = \sum_n |C_n|^2$  is the total power. The effective nonlinearity parameter is now  $\chi = \gamma P$ , and the  $\phi_n$  are normalized to unity:  $\sum_n |\phi_n|^2 = 1$ . The idea is to start from the linear embedded state with given eigenvector  $\lambda$  at  $\chi = 0$ . Then, we gradually increase or

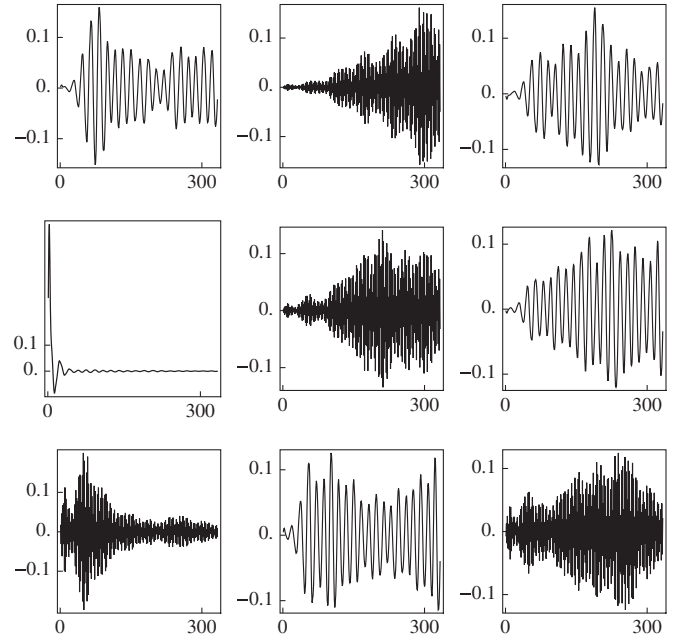


FIG. 5. Perturbed states in the continuum spectrum band that are the closest in energy to the embedded mode (left middle panel) ( $N = 333$ ,  $k = 0.33$ ).

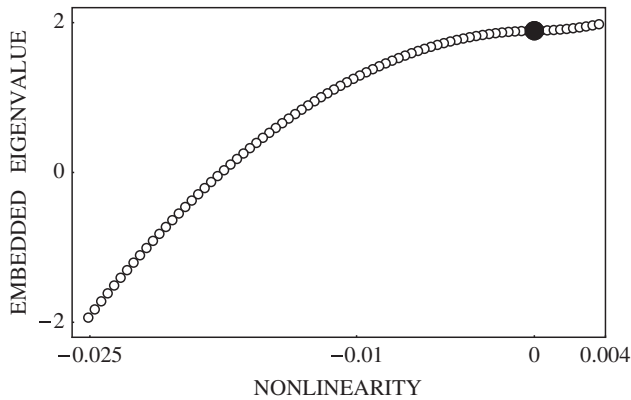


FIG. 6. Eigenvalue of the embedded surface mode as a function of the scaled nonlinearity strength  $\chi = \gamma P$ , for  $N = 133$  and  $k = 0.33$ . Black circle marks the position of the embedded eigenvalue in the absence of nonlinearity.

decrease  $\chi$  and follow the evolution of its eigenvalue and spatial profile, by solving Eqs. (12) and (13) in a self-consistent manner.

Results from this procedure are shown in Fig. 6. We see that the eigenvalue of the embedded state can indeed be tuned to occur at any value inside the band, by means of a small amount of focussing or defocussing nonlinearity. The embedded state profile does not change perceptibly during this process, as expected from the above discussion.

The procedure described above for one-dimensional semi-infinite discrete lattices could be generalized to higher dimensions. The simplest of such cases is a semi-infinite square lattice where the surface modes can exist near the edges and corners of a large square lattice. There, and given the separability of the Hamiltonian that gives rise to the evolution equations, the spatial profile of the embedded mode can be written as  $C_{n,m} = \phi_n \phi_m$ , where  $\phi_n = \sin(nk_x) f_n^x$  and  $\phi_m = \sin(mk_y) f_m^y$ , where the envelope functions  $f_n^x$  and  $f_m^y$  are the same. The eigenvalue of the embedded mode is  $\lambda = \lambda_x + \lambda_y$  and the energy site distribution is simply  $\epsilon_{n,m} = \epsilon_n + \epsilon_m$ , each is given by the appropriate modification of Eq. (6).

In summary, we have suggested and studied a novel type of bound states localized at the edge of a semi-infinite discrete lattice with the eigenvalues embedded in the continuous spectrum. We have demonstrated a procedure to generate square-integrable, surface localized modes embedded in the continuum, as well as the site energy distributions needed to produce such modes. We have shown that these new embedded modes are structurally stable, and their location inside the band can be tuned by weak nonlinearity. We believe the ideas demonstrated here may be useful in other fields, including atomic systems, quantum-confined structures, as well as a variety of photonic and phononic structures where such bound states may appear through cancellation of radiation in waveguides with side-coupled defects.

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- [1] J. von Neumann and E. Wigner, *Phys. Z.* **30**, 465 (1929).
  - [2] F.H. Stillinger, *J. Chem. Phys.* **45**, 3623 (1966); F.H. Stillinger and T.A. Weber, *Phys. Rev. A* **10**, 1122 (1974); F.H. Stillinger and D.E. Stillinger, *Phys. Rev. A* **10**, 1109 (1974); F.H. Stillinger and D.R. Herrick, *Phys. Rev. A* **11**, 446 (1975).
  - [3] A.K. Jain and C.S. Shastri, *Phys. Rev. A* **12**, 2237 (1975).
  - [4] F. Capasso, C. Sirtori, J. Faist, D.L. Sivco, S.-N.G. Chu, and A.Y. Cho, *Nature (London)* **358**, 565 (1992).
  - [5] D.C. Marinica, A.G. Borisov, and S.V. Shabanov, *Phys. Rev. Lett.* **100**, 183902 (2008).
  - [6] E.N. Bulgakov and A.F. Sadreev, *Phys. Rev. B* **78**, 075105 (2008).
  - [7] N. Moiseyev, *Phys. Rev. Lett.* **102**, 167404 (2009).
  - [8] Y. Plotnik, O. Peleg, F. Dreisow, M. Heinrich, S. Nolte, A. Szameit, and M. Segev, *Phys. Rev. Lett.* **107**, 183901 (2011).
  - [9] E.N. Bulgakov and A.F. Sadreev, *Phys. Rev. B* **80**, 115308 (2009); E.N. Bulgakov and A.F. Sadreev, *Phys. Rev. B* **81**, 115128 (2010).