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We derive analytical solutions for the zero-energy states of degenerate shell obtained as a singular eigenvalue problem found in tight-binding (TB) Hamiltonian of triangular graphene quantum dots with zigzag edges. These analytical solutions are in agreement with previous TB and density-functional theory results for small graphene triangles and extend to arbitrary size. We also generalize these solutions to trapezoidal structure which allow us to study bowtie graphene devices.

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Low-dimensional graphene nanostructures are promising candidates as building blocks for future nanoelectronic applications due to their band gaps and magnetic properties tunable with size and shape.1–6 Remarkable progress has been made in cutting graphene sheets into nanostructures with desired shape and size, significantly influencing their properties.5,7 In particular, the existence of a band of degenerate states near Fermi level localized at the edges in zigzag ribbons8–10 and triangular dots11–17 was predicted by tight-binding model and confirmed by density-functional theory calculations. These zero-energy edge states play important role due to their large contribution to the density of states.11,14,18 In triangular graphene quantum dots, numerical results show that the degeneracy of the band of zero-energy states is proportional to the edge size and can be made macroscopic. This opens up the possibility to design a strongly correlated electronic system as a function of filling of the shell, in analogy to the fractional quantum Hall effect.17

While the existence of zero-energy states was predicted analytically for zigzag ribbons,8 for triangular structures, the analysis of zero-energy states was limited to numerical techniques such as tight-binding and density-functional theory for specific and small sizes of quantum dots. A size-independent general analytical analysis is therefore desirable. In this work, we present analytical solutions to zero-energy edge states in graphene triangles with zigzag edges. We also show how the results can be generalized to the trapezoidal structures and applied to the bowtie structures.19 Our method allows the prediction of the number of zero-energy states as a function of the size in all triangular, trapezoidal, and bowtie structures.

Our starting point is the nearest-neighbor tight-binding model. It has been successfully used to describe graphene lattice20 and applied to other graphene materials such as nanotubes, nanoribbons, and quantum dots.8,9,11–15,21 The Hamiltonian is written as

\[ H = t \sum_{\langle i,j \rangle} a_i^\dagger a_j, \]

where \( t \) is hopping integral, \( a_i^\dagger \) and \( a_i \) are creation and annihilation operators on a site \( i \) respectively, and \( \langle i,j \rangle \) indicate summation over nearest neighbors. It is important to distinguish between two types of atoms which appear in the unit cell of the honeycomb lattice of graphene sheet. For triangular structures, these atoms form two nonequivalent sublattices (A and B) and they are indicated by red (light gray) and blue (dark gray) circles of the graphene triangle in Fig. 1. Our goal is to find zero-energy solutions to the singular eigenvalue problem,

\[ H \Psi = 0. \]

In this case there is no coupling between two sublattices and the solutions can be written separately for A-type and B-type atoms as \( \Psi^\mu = \sum c_i \phi_i^\mu \) with \( \mu = A, B \). The coefficients \( c_i \) obey

\[ \sum_{\langle i,j \rangle} c_i = 0, \quad (1) \]

where the summation is over \( i \)th nearest neighbors of an atom \( j \). In other words, the sum of coefficients around each site must vanish.8 Let us first focus on the sublattice labeled by \( A \), represented by red (light gray) circles in Fig. 1. We label each atom by two integer numbers \( n \) and \( m \) (with \( 0 \leq n, m \leq N+1 \), where \( N \) is the number of A-type atoms on the one edge). The dash lines and open circles indicate auxiliary atoms which will later help to introduce boundary conditions. We will now show that coefficients \( c_{n,m} \) for all atoms in the triangle can be expressed as a linear combination of coefficients corresponding to atoms on one edge, i.e., \( c_{n,0} \). Starting from the first row and using Eq. (1), we can obtain all coefficients corresponding to atoms in the second row. For the first two coefficients from the left we obtain \( c_{0,1} = -(c_{0,0} + c_{1,0}) \) and \( c_{1,1} = -(c_{1,0} + c_{2,0}) \). These coefficients are just equal to the sum of two upper-lying coefficients with the minus sign. In analogy, we can write expressions for all coefficients in the second row. In the next step, coefficients in the third row are expressed as a sum of two coefficients in the second row. For first coefficient from the left in the third row we obtain \( c_{0,2} = -(c_{0,1} + c_{1,1}) = (c_{0,0} + 2c_{1,0} + c_{2,0}) \). The second and third ones will have similar form. By going down rows one by one, we can obtain all coefficients in the structure regardless of the size of the triangle. Similar to the construction of Pascal triangle,22 these coefficients can be written in a suitable form using binomial coefficients.
Here, it is important to emphasize that the only unknown are
the \( N+2 \) coefficients \( \psi_{0,0} \) from the first row; the rest
are expressed as their superpositions, as it is seen from Eq. (2).
In addition, we must use the boundary conditions; the
construction of the triangle requires vanishing of the coefficients
corresponding to auxiliary atoms in each corner (Fig. 1).
This gives three boundary conditions \( \psi_{0,0} = \psi_{N+1,0} = \psi_{0,N+1} = 0 \),
reducing the number of independent coefficients to \( N-1 \).

The same analysis can be done for \( B \)-type atoms indicated
by blue (dark gray) circles. In this case, it is convenient to
include some of boundary conditions at the beginning as
shown in Fig. 2, where we only keep coefficients belonging
to auxiliary atoms on the right edge. As a consequence, the
coefficient \( \psi_{0,0} \) determines all other coefficients in the
triangle. Since there are three auxiliary atoms (equivalently
three boundary conditions) but only one independent coefficient,
we cannot obtain any nontrivial solution. Hence, zero-
energy states can only consist of coefficients of one type
atoms—these lying on the edges. Now we can write general
form for the eigenvectors for zero-energy states in the
triangle,

\[
\psi = \sum_{n=0}^{N-1} \sum_{m=0}^{N-1-n} \left[ (-1)^m \sum_{k=0}^{m} \binom{m}{k} c_{n+k,0} \right] \phi_{n,m},
\]

where \( N \) is the number of atoms on the one edge and \( \phi_{n,m} \) is
\( p_z \) orbital on \( A \)-type site \((n,m)\). In this expression the only
\( N-1 \) coefficients corresponding to atoms from the first row
are independent. Thus, we can construct \( N-1 \) linearly independent
eigenvectors which span the subspace with zero-
ergy states. This is in agreement with Ref. 14—the number
of zero-energy states in the triangle is \( N-1 \), where \( N \) is
the number of atoms on one edge.

Using the Eq. (3) we can then construct an orthonormal
basis for zero-energy states. First, with the help of the three
boundary conditions, we make a choice for the \( N-1 \) inde-
pendent coefficients \( c_{n,0} \), from which we obtain \( N-1 \) linearly
independent vectors, for instance, by choosing only one non-
zero coefficient for all \( N-1 \) collections, different one for
each eigenvector. Resulting eigenvectors can then be or-
thogonalized using standard Gram-Schmidt process. The last
step is the normalization \( K_{\text{norm}} \) of the eigenvectors, using
expression

\[
K_{\text{norm}} = \sum_{n=0}^{N+1} \sum_{m=0}^{N+1-n} \left[ \sum_{k=0}^{m} \binom{m}{k} c_{n+k,0} \right] \phi_{n,m}.
\]

The method for obtaining zero-energy eigenfunction
eigencoefficients for the triangular structures can also be applied to
trapezoidal structures [inset of Fig. 3(b)]. As explained
above, the value of the coefficients for atoms in a given row
is sufficient to determine the coefficients for atoms in the
lower-lying row. If we stop this process of going down the
ladder one by one at any row, we then obtain a trapezoidal
structure. Equation (3) takes the following form:

\[
\Psi = \sum_{n=0}^{N+1} \sum_{m=0}^{N-1-n} \left[ (-1)^m \sum_{k=0}^{m} \binom{m}{k} c_{n+k,0} \right] \phi_{n,m},
\]

where \( M = \min(N+1-n, N_{\text{row}}-1) \) and \( N_{\text{row}} \) is the number of
rows in the structure [see Fig. 3(b)]. In this case the last row
contains \( N-N_{\text{row}}+2 \) auxiliary atoms which increases the
number of boundary conditions. The number of zero-energy
states is then given by \( N_{\text{row}}-2 \) (for \( N_{\text{row}}>1 \)). Here we note
that similar to the triangle, zero-energy states consist of only
one type of atoms; the only difference is increased number of
boundary conditions. In Fig. 3(a) we show tight-binding
single-particle states for triangle with \( N=5 \) atoms on one
edge. As expected, there are four zero-energy states. For comparison, in Fig. 3(b) we show single-particle states for trapezoid with the same number of atoms in a first row. Here, there are only two zero-energy states in agreement with our analysis—increasing number of boundary conditions decrease number of zero-energy states. We note that the structure which consists of only two rows (the single chain of benzene rings, called acene) does not have zero-energy states while the triangular structure with \( N \) atoms on the one edge has maximal number of zero-energy states equal to \( N-1 \). All intermediate structures (trapezoidal structures) have number of zero-energy states in the range between 1 and \( N-2 \), depending on the number of rows.

Finally we note that the solutions of Eq. (4) can also be applied to bowtie structures.19 These can be treated as two trapezoidal structures connected by their shorter base, shown in Fig. 4. It is important to emphasize that the upper trapezoid has one zero-energy state which consists of \( A \)-type atoms [red (light gray) circles] while lower trapezoid has one zero-energy state which consists of \( B \)-type atoms [blue (dark gray) circles]. Connecting these two systems does not affect the zero-energy solutions since coefficients belonging to connecting atoms are zeros. Using zero-energy eigenvectors for trapezoids, Eq. (4), we obtain expressions for two groups of zero-energy states in the bowtie structures,

$$
\Psi_A = \sum_{n=0}^{N+1} \sum_{m=0}^{M} \left[ (\pm 1)^{m} \sum_{k=0}^{m} \binom{m}{k} c_{n+k,0} \right] \phi_{n,m}^A \tag{5}
$$

for upper trapezoid, where \( A \) indicates \( A \)-type atoms from upper part and

$$
\Psi_B = \sum_{n=0}^{N'+1} \sum_{m=0}^{M'} \left[ (-1)^{m} \sum_{k=0}^{m} \binom{m}{k} c_{n+k,0}' \right] \phi_{n,m}^B \tag{6}
$$

for lower one, where \( B' \) indicates \( B \)-type atoms from lower part. Two parts of the bowtie structure are separated by the dash line in Fig. 4. Coefficients \( c_{n,0} (c_{n,0}') \) correspond to \( N \)-type (\( N' \)-type) atoms from the highest (lowest) row in the bowtie structure from Fig. 4. Note that it is possible to use Eqs. (5) and (6) to asymmetric bowtie structures consisting of two different trapezoids (\( N \neq N' \)).

In summary, we derived here analytical expression for zero-energy states in triangular and trapezoidal graphene quantum-dot structures. Our method allows prediction of the number of zero-energy states in quantum dots of arbitrary size which can be understood in terms of a competition between the number of independent coefficients and the number of auxiliary atoms (the number of boundary conditions). We also showed that the number of zero-energy states can be controlled by changing the number of rows in the trapezoidal structures but does not depend on the number of atoms in the base of the trapezoid. Finally, we applied our results to bowtie structures and showed that two independent groups of zero-energy states coexist in these systems.

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