Edge states, entanglement entropy spectra and critical hopping couplings of anisotropic honeycomb lattices

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Abstract – For bipartite honeycomb lattices, we show that the Berry phase depends not only on the shape of the system but also on the hopping couplings. Using the entanglement entropy spectra obtained by diagonalizing the block Green’s function matrices, the maximally entangled states with the eigenvalue $\lambda_m = 1/2$ of the reduced density matrix are shown to have one-to-one correspondences to the zero-energy states of the lattice with open boundaries. The existence of these states depends on the Berry phase. For systems with finite bearded edges along the $x$-direction, we show that new maximally entangled states (zero-energy states) appear pair-by-pair when one increases the hopping coupling $h$ over the critical values $h_c$’s.

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Experimental studies on graphene [1] and cold atoms [2] have generated new interests in the quantum properties of electrons and atoms in honeycomb lattices. Due to its peculiar energy dispersion, with two Dirac points as Fermi surfaces, the honeycomb lattice offers particular physical phenomena which cannot be observed in the square lattice. In particular edge states with zero energy may appear when special boundaries are present. The existence of these edge states relies on the shape of the boundaries. For zigzag and bearded edges there exist zero-energy edge states. On the contrary the armchair edges offer no zero-energy edge modes. The difference between these cases can be understood by considering the Berry phase of the occupied band [3]. Therefore the existence of zero-energy edge modes depends on the topological information of the energy bands.

On the other hand, a recent development in quantum information theory applied to condensed matter systems provides a new tool to investigate physical phenomena [4]. Especially the entanglement entropy: $S_A \equiv -\lambda_m \log_2 \lambda_m - (1 - \lambda_m) \log_2 (1 - \lambda_m)$, (1) contains global information about the system, the entanglement entropy spectra offer a new method to observe more microscopic quantum phenomena.

In this letter we explore the bipartite entanglement entropy spectra of tight-binding honeycomb lattices with different shapes of the system $A$, as shown in fig. 1. We show that not only the types of edges but also the hopping couplings $h$ along the $x$-direction influence the
Berry phase $\chi$, the value of which decides if the system has maximally entangled states with $\lambda_m = 1/2$ or not [8]. In the previous literature, only the edges with infinite length have been studied [3]. In this letter we analytically and numerically study edges with finite sizes. For bearded edges, extra maximally entangled states appear two-by-two when the hopping coupling $h$ increases through the critical values $h_c$'s. These results are verified numerically using the entanglement entropy spectra by diagonalizing the block Green’s function matrix.

We consider honeycomb lattices with anisotropic hopping constants as shown in fig. 1. The hopping coupling along the $y$-direction is defined as $2$ in magnitude, while the other two couplings are replaced by general values $h$. Without changing the lattice topology, a honeycomb lattice can be transformed into a brick-type lattice [9], therefore the Hamiltonian can be rewritten as

$$\mathcal{H} = - \sum_{k \in BZ} \left\{ t_{x,y}^c c_{x,y}^\dagger c_{x+1,y} + 1 + (-1)^{x+y} \right\} c_{x,y}^c c_{x+1,y+1} + \text{h.c.} \right\}.$$  

The dispersion relation for this Hamiltonian is: $\varepsilon(k) = 2(1 + h^2 \cos^2 k_x + 2h \cos k_x \cos k_y)^{1/2}$. For $0 < h < 1$, the system is gapped, while for $h > 1$ we find two Dirac Fermi points located at $(k_x, k_y) = (\pm \cos^{-1}(-1/h), 0)$. For $h = 1$, the two Dirac zero-energy modes merge into a confluent point $(k_x, k_y) = (\pi, 0)$. The zero-energy edge states for bearded edges appear only if the bulk has two Dirac points. The reason is described as follows.

The edges on the honeycomb lattice can be produced by imposing different open boundaries: bearded, zigzag or armchair edges. To further see the influence of the boundaries, the sublattices $\gamma$ and $\delta$ can be first labeled as $\phi$ and $\bullet$ in fig. 1. Defining a pair of annihilation operators $c_{x,y}^\dagger = (c_{x,y}, c_{x,y}^*)$ and Fourier transforming the Hamiltonian (2), we can rewrite the Hamiltonian (2) in the momentum space as

$$\mathcal{H} = - \sum_{k \in BZ} \sigma_{x,y} c_{x,y}^\dagger c_{x,y}.$$  

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and $R(k) = (R_x, R_y, R_z) \in \mathbb{R}^3$. If we consider systems without onsite potentials, one can always rotate $R(k)$ to lie on a two-dimensional plane by applying a global SO(3) unitary transformation, thus one can define $R(k) \equiv (R_x, R_y)$. With this parametrization, the energy $\varepsilon(k) = \pm |R|$. The form of $R(k)$ depends on the choice of the unit cell used in the Fourier transformation along the edges [3]. (a) For a bearded edge along the $x$-direction, $R(k) = (h[\cos k_x + \cos(k_x - k_y)] + 2, h[\sin k_y - \sin(k_x - k_y)]); (b)$ for a zigzag edge along the $x$-direction, $R(k) = (2 \cos(k_x - k_y) + 1 + \cos k_y, h[\sin k_x - 2 \sin(k_x - k_y)])$; (c) for an armchair edge along the $y$-direction, $R(k) = (h[\cos k_x + \cos(k_x + k_y)] + 2, h[\sin k_x + \sin(k_x + k_y)])$. The choice of the unit cell used in the Fourier transformation is not unique. However, different choices lead to the same topology for the bands and hence edge states. By fixing the wave vector parallel to the edges and investigating the loop of $R$ as a parameter of the perpendicular wave vector changing from $-\pi$ to $\pi$, the topology of the system can be obtained.

In case where the loop $\ell$ of $R$ encloses the origin $O$ in the $R$ space, the Berry phase (or Zak’s phase) $\chi$, defined as a line integral of the curvature of the filled band, is $\pi$. In this case, due to the fact that one can continuously deform $\ell$ into a unit circle without crossing the origin, topological argument ensures that the original Hamiltonian corresponding to $\ell$ contains at least one zero-energy edge state [3]. Therefore for (a) bearded edges along the $x$-direction, for a fixed $k_x$ and $k_y$ serving as the parameter of the loop, there exists a zero-energy state only if $-2 \cos^{-1}(1/h) \leq k_y \leq 2 \cos^{-1}(1/h)$. A similar situation happens for (b) zig-zag edges. Zero-energy edge states appear under the condition $-\pi \leq k_x \leq -\cos^{-1}(2/h^2 - 1)$ or $\cos^{-1}(2/h^2 - 1) \leq k_x \leq \pi$. On the other hand, for (c) armchair edges, no zero-energy states exist due to the fact that no loops will encircle $O$ with fixed $k_y$ by changing $k_x$. Therefore for the zigzag and bearded edges the hopping coupling $h$ changes the range of $k_x$ where the Berry phase $\chi = \pi$.

The consideration for entanglement entropy is somehow different: we no longer have a system with an open boundary, but partition it into two parts: system $A$ and environment $B$. By using von Neumann entropy $S_A$, one can figure out how the system $A$ entangles with the environment $B$. However, there exist one-to-one correspondences between the zero-energy states for the Hamiltonian with edges and the maximally entangled states for the bipartite
system. The reason is as follows. Consider the whole bipartite AB consisting of N sites (or modes), with n sites for system A. Notice that the thermodynamic limit (N → ∞) will be taken. The reduced density matrix $\rho_A = \text{Tr}_B \rho_0$, where $\rho_0 = |\Psi_{AB}\rangle \langle \Psi_{AB}|$, can be obtained by determining the matrix elements of the full density matrix with respect to coherent states and integrating out the variables of the environment B [7]. $\lambda_m$’s in eq. (1) are given by the eigenvalues of the block Green’s function matrix [10] $G_{\gamma\delta}(r_i - r_j) = \text{Tr} \rho_C(r_i, \gamma) c_i^{\dagger}(r, \delta)$, where $(r_i, \gamma)$ and $(r_j, \delta)$ belong to system A. The entanglement entropy therefore takes the same form as eq. (1). The Green’s function matrix can be Fourier transformed as $G_{\gamma\delta}(r_i - r_j) = N^{-1} \sum_{k \in BZ} e^{-i k \cdot (r_i - r_j)} G_{\gamma\delta}(k)$, where $G_{\gamma\delta}(k)$ is given by

$$G_{\gamma\delta}(k) = \frac{1}{2} \left[ 1 - \frac{R \cdot \sigma}{R} \right]_{\gamma\delta} \quad (4)$$

We can regard $G_{\gamma\delta}(r_i - r_j)$ as an effective Hamiltonian for obtaining the entanglement spectrum. In the case of taking the whole infinite plane, i.e. no sites in the environment B, the $G$ Hamiltonian has the same set of eigenfunctions as the original Hamiltonian. However, the eigenvalues are either 1 or 0, which means $S_A = 0$, the system is not entangled at all. On the other hand, when $B$ is empty, the nontrivial boundary states appear, with eigenvalues neither 1 nor 0. These boundary states, whose eigenvalues satisfy $0 < \lambda_m < 1$, give rise to nonzero entanglement entropy, therefore we can say that these are the most important states contributing to the entanglement.

The Hamiltonians (3) and $G_{\gamma\delta}(k)$ (4) almost take the same form except for a constant and a positive normalization factor $R$. Therefore we can conclude that they should share the same topology, that is, if $R$ encloses the origin in the parameter space so that the Berry phase is equal to $\pi$, then a zero-energy state appears for the Hamiltonian (3), while for the block Green’s function matrix we obtain one special eigenvalue $\lambda_m = 1/2$ [8]. They also share the same eigenfunction though with different eigenvalues. We call the state with $\lambda_m = 1/2$ a maximally entangled state due to the fact that the resulting $S_m = 1$. According to the discussions above, only the reduced density matrices of the systems A with bearded and zigzag edges have maximally entangled eigenstates, while for the armchair edges there are no maximally entangled states.

In order to investigate this effect we numerically diagonalize the block Green’s function matrix $G_{\gamma\delta}(r_i - r_j)$ for the system A with finite sizes, as shown in fig. 1, where $L_x$ and $L_y$ are defined as follows. Transforming the honeycomb lattice into the brick-type lattice and projecting the system sites into the $x$- and $y$-direction, $L_x$ ($L_y$) is defined as the total number of the projected sites along the $x$ ($y$) direction. Real noninteracting edge states only appear in the thermodynamic limit, i.e. $L_x \gg L_y$ or vice versa. For example the partitions $A_{br}$ and $A_{zz}$ in fig. 1 have either two bearded ($A_{br}$) or zigzag ($A_{zz}$) edges. On the other hand there exist two armchair edges for the system $A_{ar}$. Here we only consider the edges far apart from each other so that the two edges do not interact with each other (independent edges). Therefore we expect that for the partitions $A_{br}$ or $A_{zz}$ there exist maximally entangled states ($\lambda_m = 1/2$), while for $A_{ar}$ maximally entangled states do not appear. (Due to the fact that bearded and zigzag edges have the same properties, we shall only calculate the entanglement spectra for the bearded edges in the following.) The upper panels of fig. 2 show the entanglement spectra $\lambda_m$ of (a) $L_x = 3$, $L_y = 200$ ($A_{br}$-type) and (b) $L_x = 201$, $L_y = 4$ ($A_{ar}$-type) for a graphene ($h=2$). For the system with two independent bearded edges, we obtain two maximally entangled states with $\lambda_m = 1/2$ (see the inset), while there are no maximally entangled states for the system with $L_x \gg L_y$ (right-hand side of fig. 2) due to the fact that the $A_{ar}$-type system has two independent armchair edges. Figure 2(c) shows the spectra for $L_x = 11$, $L_y = 200$ and $h = 2$. From the inset we observe 6 eigenvalues close to 1/2. In fig. 2(d) the system size is the same as (c) but the hopping coupling $h = 4$. We obtain 10 maximally entangled states (due to the finite-size effect, two eigenvalues of the states are not precisely 1/2, however we still count them as maximally entangled states). The number of maximally entangled states not only depend on the shape of the system but also on the hopping coupling $h$. We shall discuss this as follows.

For general $h$, the wave functions of a maximally entangled state is the same as the corresponding zero-energy mode. A zero-energy wave function is obtained by solving the tight-binding Schrödinger equation (SE) $-\sum_j t_j \psi_j = E \psi_i = 0$, where $j$ are neighboring sites.
of \( i \), \( t_j = \hbar \) for the horizontal hopping couplings and \( t_j = 2 \) for the vertical hopping constants in the brick-type representation. Figure 3(a) shows the structure of the system with \( L_y \gg L_x = 3 \). To obey the SE, a solution with all values of the wave function for the \( \alpha \)-sites in fig. 3 equal to zero is expected. Solutions can further be divided into two groups, with symmetric or antisymmetric wave functions with respect to the midline of the system along the \( y \)-direction. For symmetric solutions, we set \([\psi_A, \psi_B] = [\phi, \phi]\). According to the SE, \( \psi_B = -(2/\hbar^2)\phi \) and \( [\psi_{C_1}, \psi_{C_2}] = [(2/\hbar^2)\phi, (2/\hbar^2)\phi] \). Therefore there exist maximally entangled states (zero-energy states) only if \( 2/\hbar^2 < 1 \), otherwise the wave function will explode with the increasing \( L_y \). We obtain a critical \( h_c = \sqrt{2} \): the maximally entangled states appear only if \( h \geq h_c \). On the other hand, the antisymmetric solutions \([\psi_A, \psi_B] = [\phi, -\phi]\) fail for \( L_x = 3 \) due to the fact that the value on site \( B_1 \) directly sets \( \phi = 0 \).

Another example we study here is \( L_x = 11 \), as shown in fig. 3(b). For the symmetric wave functions, we can first set the values \([\psi_A] = [1, \alpha_1, \alpha_2, \alpha_2, \alpha_1, 1]\) and \([\psi_B] = [\beta_1, \beta_2, \beta_3, \beta_3, \beta_1, \beta] \phi \). Due to the fact that the structure of the layer \( C_1 \) is the same as \( A_1 \), the values of the wave function can be set as \( [\psi_{C_1}] = x[\psi_A] \). To obtain the critical couplings \( h_c \)’s we have to know all these values \( \alpha_1, \beta_1, x \) by using the SE at different \( \alpha \)-sites. The SE for the site between \( A_1 \) and \( B_1 \) gives \( \beta_1 = -2/\hbar \). The site among \( A_2 \), \( B_1 \) and \( B_2 \) leads to the equation \( \beta_2 = 2(1-\alpha_1)/\hbar \). In the same manner we obtain \( \beta_3 = 2(\alpha_2-\alpha_1-1)/\hbar \). Using these relations and the SE for the \( \alpha \)-site between \( B_2 \) and \( C_2 \), the first value for \( x \) is found: \( x = 4/(1+\alpha_1)^2 \). From this relation the critical coupling is obtained by setting \( x = 1 \), i.e. \( h_c = 2/\sqrt{1+\alpha_1} \). \( h_c \) is therefore obtained if \( \alpha_1 \) is known. On the other hand, different relations for \( x \) can be obtained by subsequently calculating the SE for the \( \alpha \)-sites among \( B_1 \) and \( C_1 \): \( x = 4(\alpha_1-1)/[(\alpha_1+\alpha_2)\hbar^2] \) and \( x = 2(1+\alpha_2-\alpha_1)/(\alpha_2\hbar^2) \). These three \( x \)'s should be identical, we first obtain \( \alpha_2 = \alpha_1^2 - \alpha_1 - 1 \) and finally the polynomial for \( \alpha_1 \) is found: \( \alpha_1^3 - 3\alpha_1^2 + 2 = 0 \). This indicates that \( \alpha_1 = 1 \) or \( \alpha_1 = 1 \pm \sqrt{3} \). For the symmetric eigenfunctions we obtain three critical couplings \( h_c = \sqrt{2}, 2\sqrt{2} - \sqrt{3} \) and \( 2\sqrt{2} + \sqrt{3} \) corresponding to the different \( \alpha \)-s.
$L_x = 3$ can build a system with $L_x = 7$; a sandwich-like system with two $L_x = 3$ positive blocks on both sides and a negative block in the middle has exactly the size $L_x = 11$. Similarly, for $L_x = 5$ and $L_x = 11$ there exists the same $h_c = 2$. It is clear that a positive and a negative block with $L_x = 5$ can build a system with $L_x = 11$.

An interesting question arises: if we consider now a system with onsite potentials, i.e., with $R = (R_x, R_y, R_z)$, $R_z = \Delta$, do the edge states still robustly exist? By adding the onsite potentials, the chiral symmetry is destroyed, there do not exist maximally entangled states. The blue lines and dots of the inset in fig. 2 show the small deviation of $\lambda$ from $1/2$ when $\Delta = 0.01$. However, due to the fact that the deviation is small, we can conclude that the states with eigenvalues close to $1/2$ are still edge states. That means, the edge states robustly exist even with broken chiral symmetry.

In summary, we have used the entanglement spectra to study the edge states of a honeycomb lattice. The relation between the Berry phase and hopping couplings has been found. The one-to-one correspondence between the maximally entangled state for a bipartite system and the zero-energy state has been proven numerically by diagonalizing the block Green’s function matrix. We found there exist critical couplings $h_c$’s for the system with finite edges: additional maximally entangled states appear pair-by-pair every time when $h$ increases over a set of critical values $h_c$’s.

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