Exact wave functions for the edge state of a disk-shaped two dimensional topological insulator

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We report the exact wave functions for the eigen state of a disk-shaped two dimensional topological insulator. The property of the edge state whose energy lies inside the bulk gap is studied. It is found that the edge state energy is affected by the radius of the disk. For a fixed angular momentum index, there is a critical disk radius below which there exists no edge state. The value of this critical radius increases as the angular momentum index increases. In the limit of large disk radius, the energy of the edge state approaches a limiting value determined by the system parameters and independent of the angular momentum index. The derivation from this limiting value is inversely proportional to the radius with a coefficient proportional to the angular momentum index. In the general case, the energy differences between two edge states with adjacent angular momentum indexes are not equal. The exact and analytical wave functions also facilitates the investigation of electronic state in other structures of the two dimensional topological insulator.

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Topological insulator has attracted considerable attentions in recent years [1–3]. In two dimensions, the topological insulator is described by an effective model [4]. Many theoretical investigations into the exotic properties of two dimensional topological insulator (2DTI) are based on this model [4].

Despite those great progresses achieved, exact wave function for the 2DTI is rarely reported so far. When a 2DTI is cut into a ribbon like structure, exact wave functions were obtained [5]. It is found that due to the finite width of ribbon, there is a gap in the energy spectrum which decreases exponentially as the width of the ribbon increases [5].

In the present paper, we report exact wave functions for the 2DTI with a circular geometry. This allows us to probe some exact properties of 2DTI. In particular, we focus on the edge state of a disk shaped 2DTI with the open boundary condition that both components of wave functions vanish at the disk edge. The electronic state in other geometric structure will also be briefly discussed.

The 2DTI is described by the following well-known Hamiltonian [4]

\[
\begin{pmatrix}
h(k) & 0 \\
0 & h^*(k)
\end{pmatrix},
\]

where \( k = (k_x, k_y) \), \( h(k) = \epsilon(k) + \sum_{\sigma} \sigma_\alpha d_\alpha(k) \sigma_\alpha \) with \( \sigma_\alpha \) the Pauli matrix. \( \epsilon(k) = C - D(k_x^2 + k_y^2) \), \( d_1 = Ak_x \), \( d_2 = Ak_y \), and \( d_3 = M - B(k_x^2 + k_y^2) \). \( A, B, C, D, \) and \( M \) are parameters determined by the structure of the quantum well [4]. Operators \( k_x \) and \( k_y \) represent differential operators \( -i\partial_x \) and \( -i\partial_y \) respectively. The parameter \( C \) gives the zero point of energy and we can safely set it to zero for simplicity in this paper. The spin-up block \( h(k) \) and spin-down block \( h^*(k) \) in the Hamiltonian are decoupled and they can be solved separately [4]. Since the the system under consideration has a circular geometry, we will adopt the polar coordinate system. It can be shown that the radial and angular part of the wave function can be separated. This simplifies the problem and one only needs to solve the radial wave function.

For the spin-up block \( h(k) \), the wave function can be written as

\[
\Phi_m(r, \theta) = \begin{pmatrix}
\phi_1(r) \\
\phi_2(r)
\end{pmatrix} = \begin{pmatrix}
C_1 Z_m(\lambda r) \\
C_2 Z_{m+1}(\lambda r)
\end{pmatrix},
\]

where \( m = 0, \pm 1, \pm 2, \pm 3, \ldots \) is the angular momentum index. The differential equations for the radial part can be written as

\[
\begin{pmatrix}
O_m + X_1 & X_3 P_{m+1} \\
X_4 P_m - O_{m+1} + X_2
\end{pmatrix}
\begin{pmatrix}
\phi_1(r) \\
\phi_2(r)
\end{pmatrix} = 0,
\]

with \( O_m = d^2/dr^2 + d/dr - m^2/r^2, P_m = d/dr + m/r, X_1 = (-E + V(r) + M)/(B + D), X_2 = (E - V(r) + M)/(B - D), X_3 = -iA/(B + D), \) and \( X_4 = iA/(B - D). \) \( E \) is the energy of the system and \( V(r) \) the externally applied potential that depends only on the radial coordinate.

In this paper, we consider \( V(r) \) taking different but constant values in the different regions of \( r \). In this case, the exact wave function can be written as

\[
\Phi_m(\lambda r) = \begin{pmatrix}
\phi_1(r) \\
\phi_2(r)
\end{pmatrix} = \begin{pmatrix}
C_1 Z_m(\lambda r) \\
C_2 Z_{m+1}(\lambda r)
\end{pmatrix},
\]

with \( Z_m(\lambda r) \) the Bessel functions \( J_m(\lambda r) \) or \( Y_m(\lambda r) \). \( \lambda, C_1, \) and \( C_2 \) are solution of a secular equation

\[
\begin{pmatrix}
X_1 - \lambda^2 & X_3 \lambda \\
-4 X_4 \lambda & X_2 - \lambda^2
\end{pmatrix}
\begin{pmatrix}
C_1(\lambda) \\
C_2(\lambda)
\end{pmatrix} = 0.
\]

The equation gives four roots of \( \lambda: \pm \lambda_1 \) and \( \pm \lambda_2 \), as

\[
\lambda_1 = [(F + \sqrt{F^2 - 4X_1 X_2})/2]^{1/2}, \quad \lambda_2 = [(F - \sqrt{F^2 - 4X_1 X_2})/2]^{1/2},
\]

with \( F = X_1 + X_2 - X_3 X_4 \). Note that \( \lambda \) is a function of potential \( V \) and energy \( E \). \( C_1 \) and \( C_2 \) are only determined up to factor.
The value of $\lambda$ obtained in Eq. (6) can become imaginary. In that case, it is more convenient to write the exact wave function as

$$\Phi_m(\xi r) = \left( \begin{array}{c} \phi_1(r) \\ \phi_2(r) \end{array} \right) = \left( \begin{array}{c} C_3 Z_m(\xi r) \\ C_4 Z_{m+1}(\xi r) \end{array} \right),$$  \hspace{1cm} (7)

with $Z_m(\xi r)$ the Bessel functions $I_m(\xi r)$ or $(-1)^m K_m(\xi r)$. $\xi$, $C_3$, and $C_4$ are solution of a secular equation

$$\begin{pmatrix} X_1 + \xi^2 & X_3 \xi \\ X_4 \xi & X_2 + \xi^2 \end{pmatrix} \begin{pmatrix} C_3(\xi) \\ C_4(\xi) \end{pmatrix} = 0.$$  \hspace{1cm} (8)

The equation gives four roots of $\xi$: $\pm \xi_1$ and $\pm \xi_2$, as

$$\xi_1 = \left[ -F + \sqrt{F^2 - 4X_1X_2} \right]/2^{1/2},$$

$$\xi_2 = \left[ -F - \sqrt{F^2 - 4X_1X_2} \right]/2^{1/2},$$

with $F = X_1 + X_3 - X_4$ the same as given before. The $E$ dependence of $\xi$ in Eq. (9) depends also on other model parameters. With the parameters given in Eq. (4), one can readily verify that when $|E - V| < |M|$, both $\xi_1$ and $\xi_2$ are real and non-zero. When $|E - V| = |M|$, $\xi_1$ is non-zero and real, and $\xi_2 = 0$. When $|E - V| > |M|$, both $\xi_1$ and $\xi_2$ are non-zero, $\xi_1$ remains real, and $\xi_2$ is purely imaginary.

It can be shown that $\Phi_m(\lambda r)$ and $\Phi_m(-\lambda r)$ (or $\Phi_m(\xi r)$ and $\Phi_m(-\xi r)$) are not linearly independent solutions. Therefore we have linearly independent solutions $\Phi'_m(\lambda r)$ and $\Phi''_m(\lambda r)$, or $\Phi'_m(\xi r)$ and $\Phi''_m(\xi r)$. The superscripts $J$, $Y$, $I$, and $K$ denotes the kind of the Bessel functions involved. The desired wave function can be constructed as a linear combination of the linearly independent solutions. In the case of $\lambda = 0$ or $\xi = 0$, a careful treatment of $\lambda \to 0$ or $\xi \to 0$ limit is required in order to obtain linearly independent solutions.

For the spin-down block $h^s(-k)$, the exact wave function can be obtained in the same way. A careful examination shows that the energy of spin-up state with angular momentum index $-|m|$, denoted as $E_{-|m|,\uparrow}$, exactly equals to $E_{|m|-1,\downarrow}$ the energy of spin-down state with angular momentum index $|m| - 1$. One has $E_{-|m|,\uparrow} = E_{|m|-1,\downarrow}$ and $E_{-|m|,\downarrow} = E_{|m|-1,\uparrow}$.

Next, we use the exact wave functions obtained above to construct the edge state for a disk shaped 2DIT. In this quantum disk system, one has $V(r) = 0$ for $r < R$ with $R$ the radius of the disk. The boundary condition is that both components of the wave functions must vanish at $r = R$. When the energy falls inside the bulk gap $E^2 < M^2$, Eq. (9) gives to two real $\xi_1$ and $\xi_2$, and with model parameters given in Fig. (4), the wave functions that involve the Bessel function $K_m(\xi r)$ are divergent at $r = 0$ and must be discarded. Therefore, we construct the desired wave function from $\Phi'_m(\xi r)$ and $\Phi''_m(\xi r)$ by requiring $d_1 \Phi'_m(\xi_1 R) + d_2 \Phi''_m(\xi_2 R) = 0$, with $d_1$ and $d_2$ the coefficients to be determined. This leads to the following equation for the spin-up case

$$\begin{align*}
\xi_1(\xi_1^2 + X_1) & = I_m(\xi_1 R)I_{m+1}(\xi_1 R), \\
\xi_2(\xi_2^2 + X_1) & = I_m(\xi_2 R)I_{m+1}(\xi_2 R),
\end{align*}$$  \hspace{1cm} (10)

from which the eigen state energy can be obtained. The nature of function $I_m(\xi r)$ guarantees that the amplitude of the edge state wave function will be large near the disk edge and small in the disk center.

In the large disk radius limit, i.e. $R \to \infty$, $I_m(\xi r)$ approaches to $e^{\xi r}/\sqrt{2\pi \xi r}$, a value independent on $m$. From Eq. (10) we obtain eigen state energy $E_0 = -DM/B$ for both spin-up and spin-down states. For large radius $\xi R >> 1$, the eigen state energy is given by $E_{m,s} = E_0 + \delta E_{m,s}$ ($s$ denotes the spin index) with

$$\delta E_{m,s} \approx C'_s (m + \frac{1}{2}) R^{-1},$$  \hspace{1cm} (11)

where $C'_s$ is a factor only relies on the model parameters and spin. Eq. (11) suggests that for a large radius of the disk, the energy of the edge states approach linearly in $R^{-1}$ to the limiting value $E_0$, and for a fixed $R$ one get equal energy spacing for eigen states with adjacent $m$ index.

In general, the eigen state energy denoted as $E_{m,s}(R)$ is a function of $m$ and $R$. In Fig. 1 $E_{m,s}(R)$ is shown as a function of the angular momentum index $m$ for three values of $R$. The energy of spin-up states is depicted by solid symbols and the energy of spin-down states is shown by open symbols. The energy exhibits an approximately linear dependence on $m$ and the slope of the curves becomes smaller as the radius $R$ increases. It is found that for each $m$, there is a critical value $R^c_m \neq 0$ such that for $R < R^c_m$ no edge states can exist inside the bulk gap as one can not find any energy $|E| < |M|$ that Eq. (10) holds. It is also found that $R^c_m$ becomes larger as $m$ increases.

In Fig. 2 the energy state energy is shown as a function of $R^{-1}$ for several values of $m$. It is clear that the $R^{-1}$
dependence is not linear. For a fixed \( m \), this non-linear dependence is different for spin-up and spin-down states.

Eq. (11) shows that for large disk radius the energy dependence of the edge state energy shown in Fig.1 is non-linear intrinsically.

In the remaining part of this paper, base upon our exact wave functions, we discuss some interesting aspects of 2DTI systems with circular geometry. In the case of the disk shaped 2DTI, with the open boundary condition, one may also seek eigen state with energy outside the bulk gap. In this case, the wave function is a linear combination of \( \Phi^s_n(\lambda_1 r) \) and \( \Phi^d_n(\lambda_2 r) \). Since \( J_m(\lambda r) \) is an oscillatory function, but \( I_m(\lambda r) \) grows exponentially, the boundary condition results in a larger weight for the \( \Phi^s_n(\lambda_1 r) \) term. Thus, the amplitude of wave function can not be mainly concentrated near the edge and decay exponentially toward the center of disk.

Let us consider the anti-disk system: a hole in the 2DTI plane. The potential is given by \( V(r) = 0 \) when \( r > R \). The open boundary condition is adopted. For energy inside the bulk gap, The wave function is a linear combination of \( \Phi^K_n(\xi_1 r) \) and \( \Phi^K_n(\xi_2 r) \). The wave function will mainly concentrated near the edge, thus one has an edge state. When the energy is outside the bulk gap, the physically allowed wave function is a linear combinations of \( \Phi^K_m(\xi_1 r) \), \( \Phi^K_m(\lambda_1 r) \) and \( \Phi^K_m(\lambda_2 r) \). The boundary condition can only provide two equations, but there are three coefficients to be determined. This means that one can find an eigen state for any energy outside the bulk gap, completely different from the disk case. It is also found that for each \( m \), there is a critical value \( R^*_{m} \neq 0 \) (different from the disk case) such that for \( R < R^*_m \) no edge states can exist inside the bulk gap. It is found that \( R^*_m \) becomes larger as \( m \) increases. This indicates that, an infinite 2DTI may have no edge state though it has a finite length edge.

Next, we consider a ring-like geometry of the 2DTI, i.e., \( V(r) = 0 \) for \( R_1 < r < R_2 \), with the open boundary condition adopted for both edges. When the energy falls inside the bulk gap, wave functions are a linear combination of \( \Phi^K_m(\xi_1 r) \), \( \Phi^K_m(\xi_2 r) \), \( \Phi^K_m(\lambda_1 r) \), and \( \Phi^K_m(\lambda_2 r) \). The boundary conditions give four equations for the four coefficients to be determined. One should have a discrete energy spectrum. This system is similar to the ribbon structure [5] but the two edges are different.

Let us finally consider the case that the potential \( V(r) \) is a step function, i.e., \( V(r) = V_0 \neq 0 \) for \( r < R \), and \( V(r) = 0 \) otherwise. This system can be implemented experimentally by depositing metal gates on top of the 2DTI. As the potential \( V \) takes different values for \( r < R \) and \( r > R \), the values of \( \lambda \) in Eq. (4) or \( \xi \) in Eq. (5) will be different in the different \( r \) regions. In the following, we introduce a superscript \( < \) for \( \lambda \) and \( \xi \) in the region \( r < R \), and a superscript \( > \) in the region \( r > R \).

In the region \( r < R \), the allowed contributions to the wave functions are: (1) \( \Phi^K_m(\xi_1 r) \) and \( \Phi^K_m(\xi_2 r) \), when \( |E - V_0| < |M| \) (both \( \lambda_1^2 \) and \( \lambda_2^2 \) imaginary); (2) \( \Phi^K_m(\lambda_1 r) \) and \( \Phi^K_m(\lambda_2 r) \) when \( |E - V_0| > |M| \) (\( \lambda_1^2 \) real, \( \lambda_2^2 \) imaginary). For \( r > R \), the allowed contributions are: (1) \( \Phi^K_m(\xi_1 r) \) and \( \Phi^K_m(\xi_2 r) \) when \( |E| < |M| \) (both \( \lambda_1^2 \) and \( \lambda_2^2 \) imaginary); (2) \( \Phi^K_m(\lambda_1 r) \) and \( \Phi^K_m(\lambda_2 r) \) when \( |E| > |M| \) (\( \lambda_1^2 \) real, \( \lambda_2^2 \) imaginary). The boundary condition is that the wave function and its first order derivative should be both continuous at \( r = R \). The boundary condition now leads to four equations.

When \( E > |M| \) or \( E < -|M| \), the system should have a continuous energy spectrum, for any \( V_0 \neq 0 \). This is
because that the number of coefficients needed to be determined is larger than the number of equations due to the boundary condition. When $|E| < |M|$, the quantization of energy level is expected.

In summary, the exact wave functions for the eigen state of a disk-shaped two dimensional topological insulator is reported. The property of edge state is studied. For a fixed angular momentum index $m$, there is a critical disk radius below which the edge state is not possible. The value of this critical radius increases as $m$ increases. The $R^{-1}$ dependence of the edge state energy is non-linear. The $m$ dependence of the edge state energy is non-linear as well. The exact wave functions also make it easy for us to investigate the electronic state in other structures of the two dimensional topological insulator.

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