Band rearrangement through the 3D-Dirac equation with boundary conditions, and the corresponding topological change

December 14, 2018

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Abstract

Rearrangement of energy bands against a parameter is studied through the 3D-Dirac equation on a ball in \( \mathbb{R}^3 \) under the APS and the chiral bag boundary conditions on the boundary two-sphere, where APS is an abbreviation of Atiyah-Patodi-Singer. The notion of spectral flow and its extension is introduced to characterize the energy eigenvalue redistribution against the parameter, which reflects an analytical property of edge eigenstates. It is shown that though band rearrangement takes place the net spectral flow is zero \((1 + (-1) = 0)\) for both boundary conditions. The corresponding semi-quantum Hamiltonian defined on the 3D momentum space is studied in parallel and it is shown that a change against the parameter is observed in the mapping degree defined for the semi-quantum model Hamiltonian, which is viewed as reflecting a topological property of the bulk eigenstates of the full quantum system. Specifically, there are two mappings assigned, for which changes in mapping degree take the values \(\pm 1\). The present correspondence is viewed as a bulk-edge correspondence.

Keywords: energy band, Dirac equation, APS and chiral bag boundary conditions, mapping degree, bulk-edge correspondence

Mathematics Subject Classification 2010: 35Q41, 53C80, 81Q70, 81V55

1 Introduction

A relation between band rearrangement and topological change in quantum states or what is called the bulk-edge correspondence have been increasingly attractive in condensed
matter physics, especially in topological insulators, a review of which is found in [10, 25],
for example. It is to be recognized that among different fields of physics similar topological
ideas are shared under respective nomenclatures such as band rearrangement or energy
level redistribution, gap closing [59], gap node [23], gapless excitation, contact of the
conduction band and the valence band at a single point [1], and Dirac points [10], etc.
The authors have been interested in this theme from the viewpoint of molecular physics
[16, 35, 37, 38, 41].
A setup for pursuing this theme in molecular physics is stated as follows: There is a
class of molecular systems such that the whole set of dynamical variables can be split into
subsets associated with low- and high-energy excitations [19]. Depending on modelings,
the dynamical variables in a molecular system are separated into electronic and vibrational
variables, orbital and spin ones, or rotational and vibrational ones, to cite a few. Among
such modelings, the rotation-vibrational problem is taken as a reference problem. In
this modeling, the rotational variables describing high-density energy levels due to low-
energy excitations can be treated as classical ones which range over a two-dimensional
sphere on account of the conservation of the angular momentum, but the vibrational
variables describing high-energy excitations remain to be treated as quantum ones. Such
construction is called a semi-quantum model and can be naturally generalized to quantum
systems possessing subsystems of “slow” and “fast” variables of different nature.
Within semi-quantum rotation-vibration models, the authors have been studying band
rearrangements for isolated molecules in terms of Chern numbers in a series of papers
[35, 36, 37, 41, 16]. A family of semi-quantum Hamiltonians is defined to be Hermitian
matrices on the two-sphere along with some control parameters. Symmetry is often taken
into account, and the family of the Hamiltonians are supposed to be invariant under
a prescribed group which is a continuous or a finite subgroup of the orthogonal group
$O(3)$. For this family of semi-quantum Hamiltonians, the Chern number is defined for the
complex line bundles associated with each of non-degenerate eigenvalues. The parameter
space is divided into connected regions to every point of which the same Chern number
is assigned but the different regions have respective Chern numbers (see figures in [35]
and [37] in the presence of $D_3$ and $O$ symmetries, respectively). The boundaries between
different regions correspond to degeneracy of eigenvalues, which is responsible for the
modification of band structure. The variation in Chern numbers in crossing the boundary
between different regions is counted by means of related winding numbers and the orbit
of the symmetry group, and is shown to qualitatively explain the band rearrangement
for an isolated molecule [37, 41]. A general description of the stratification of the set of
eigenvalues and eigenvectors of a family of Hermitian matrices is found in [7, 8].
If the coupling between rotation and vibration is not weak, the simple splitting of
quantum energy levels is not available [28, 54]. Strictly speaking, rotational and vibra-
tional motions cannot be separated on the level of classical mechanics [24] and hence one
needs to set up classical and quantum mechanics in terms of fiber bundles by taking into
account the non-separability of rotation and vibration [31, 32]. In this setting, a number
of articles have been published [33, 34, 57]. Nevertheless, if a finite set of vibrational
levels can be chosen, effective model Hamiltonians for rotation-vibration systems are of
practical use to study a question as to what kinds of rearrangement of band structure are
allowed under the variation of control parameters in the presence of symmetry [38].
At this stage in Introduction, it is significant to compare the idea as to fast- and slow variables in molecular physics with bulk-edge correspondence in topological insulator theory. In the topological insulators, while the edge state is described quantum mechanically, the bulk states are allowed to be described in terms of classical variables, specifically, in the momentum variables [21, 48]. This procedure can be interpreted from the viewpoint of molecular physics as follows: The insulator is viewed as a two-band system, and the bulk-state energy levels are of high density, so that the bulk states can be treated in terms of classical variables in a semi-quantum model. Hence, the Chern number comes into sight as a topological invariant which characterizes the bands. Incidentally, a study of topological insulators has been made also under the named of bulk boundary principle [22, 50]. In particular, in [50], bulk and boundary invariants for lattice systems are studied by means of K-theory.

Interest in topological study of intersection of potential energy surfaces on the basis of Hermitian matrices dates back to [29] and led to the Berry phase [11, 12, 62]. Hermitian matrices have been effectively used [55, 63] in semi-quantum molecular models as well. The relevance of Chern numbers to band rearrangements in isolated molecules was initially suggested in [49] and studied further for formation of more concrete relation between Chern numbers and the numbers of states in the band [18, 19, 20]. As is mentioned above, a spectacular appearance of Chern numbers is made in the description of quantum Hall effect [6, 44, 58], though the base manifold of the relevant line bundle is a two-torus in contrast to the two-sphere for rotation-vibration problems for isolated molecules. Increasing interest has centered on topological phenomena such as the quantum spin Hall effect and topological insulators [42, 52, 25, 9, 10], and further attempt has been made for classifying topological phases [43, 53, 56].

In the course of the study on band rearrangement in semi-quantum models [37, 41], the authors have observed that elementary band rearrangement (or level-crossing) takes place between two adjacent bands and can be characterized by a topological invariant which can be evaluated through the linearization of the Hamiltonian at a critical point, and they have called the elementary topological change a delta-Chern. Further, they pointed out, in previous papers [39, 40], that the linearization method works well for the study of band rearrangement both in semi-quantum and full quantum models. In [39, 40], 2D Dirac equations with boundary conditions are intensively solved with interest in qualitative modifications of band structures in the full quantum model together with interest in analogous modification in the corresponding semi-quantum model. It was shown that the delta-Chern [37, 41] defined for a parametric family of Hamiltonians in the semi-quantum model corresponds to the spectral flow or its extension for the 2D Dirac equation in question, where the spectral flow of a one-parameter family of self-adjoint operators is originally defined to be the net number of eigenvalues passing through zero in the positive direction as the parameter runs [5, 51] and then extended in [40], and where the delta-Chern is a jump in the Chern number which takes place when the parameter crosses a critical value. The authors have already given non-linear two-dimensional models which exhibits the correspondence between spectral flows and changes in Chern numbers [16]. The present correspondence is, in principle, the same as the bulk-edge correspondence for topological insulators without time-reversal symmetry [21].
The one-parameter family of Dirac operators studied in [39, 40] is given by

$$H_t = -i \sum_{k=1}^{2} \sigma_k \nabla_k + t\sigma_3, \quad \nabla_k = \partial / \partial q_k,$$

(1)

where $t$ is a control parameter and where $\sigma_j$, $j = 1, 2, 3$, are the standard Pauli matrices. The eigenvalue problem for $H_\mu$ is set on the disk $q_1^2 + q_2^2 \leq R^2$ under the APS and the chiral bag boundary conditions on the circle $q_1^2 + q_2^2 = R^2$, where APS is an abbreviation of Atiyah-Patodi-Singer [5]. The corresponding semi-quantum Hamiltonian is given by replacing the operators $-i\nabla_k$ by the real variables $\xi_k$, $k = 1, 2$.

A question arises as to whether the correspondence between the spectral flow and the delta-Chern is a key, or not, to the understanding of the relation between band rearrangement and topological change, independently of a choice of models. Put in another way, the present question is as to whether the bulk-edge correspondence holds for a wider class of model Hamiltonians or not. A further way to approach the present question is to consider higher-dimensional cases. If group actions such as a time-reversal transformation with half-integer spin degrees of freedom are taken into account, then new Hamiltonians comes to be defined in dimensions larger than two, in both quantum and semi-quantum models. Another view of the extension of Hamiltonians is taken through gamma matrices. If $4 \times 4$ gamma matrices are adopted, corresponding Dirac Hamiltonians are to be defined on $\mathbb{R}^3$ or $\mathbb{R}^4$. The present paper deals with the Dirac Hamiltonian defined on $\mathbb{R}^3$ and the corresponding semi-quantum Hamiltonian, both of which admit the time-reversal and the chiral symmetries. Since the Chern number is defined for vector bundles over even-dimensional manifolds and since the manifold $\mathbb{R}^3$ on which the model Hamiltonians are to be defined is of odd-dimensions, another topological invariant should be introduced to describe a topological character. In the last section of this paper, remarks will be made on Dirac Hamiltonians defined on $\mathbb{R}^4$ together with the corresponding semi-quantum Hamiltonian.

Among several representations of the gamma matrices, the choice made in the present article is

$$\gamma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}, \quad k = 1, 2, 3, \quad \gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

(2)

where $\mathbb{1}$ denotes the $2 \times 2$ unit matrix. Then, the 3D Dirac Hamiltonian takes the form

$$H_\mu = -i \sum_{k=1}^{3} \gamma_k \nabla_k + \mu \gamma_0 = \begin{pmatrix} \mu \mathbb{1} & -i\sigma \cdot p \\ i\sigma \cdot p & -\mu \mathbb{1} \end{pmatrix}, \quad p = -i\nabla,$$

(3)

where $\mu$ is a parameter, which originally denotes the mass but is allowed to take negative values in the present study. In Dirac’s textbook [15], the alpha matrices are used in place of the gamma matrices (2), where $\alpha_k = \sigma_1 \otimes \sigma_k$, $k = 1, 2, 3$ while $\gamma_k = \sigma_2 \otimes \sigma_k$.

In order to obtain discrete energy eigenvalues for $H_\mu$, a boundary condition is required to be posed on the boundary of a bounded domain, since no external field is present. In this paper, the eigenvalue problems for $H_\mu$ are put on the ball of radius $R$ under the APS and the chiral bag boundary conditions. It will be shown that the eigenvalues for $H_\mu$ with the APS and the chiral bag boundary conditions are broken up into bulk- and edge-states eigenvalues, where the edge-state eigenvalues are responsible for band rearrangement but
the bulk-state eigenvalues form separate two bands, positive and negative. The spectral flow and its extension are defined for edge-state eigenvalues and has the value $1 + (-1) = 0$ for both boundary conditions. In spite of the zero value, the band rearrangement takes place indeed.

From the viewpoint of energy level density, it is shown that the difference between adjacent two bulk-state energy levels is inversely proportional to the radius of the ball, so that the bulk-state eigenvalues become of high density for a sufficiently large $R$. Hence, the bulk-state bands are allowed to be treated in terms of classical variables or in momentum variables. Accordingly, the quantum Hamiltonian $H_a$ turns into a semi-quantum Hamiltonian by replacing the classical momentum variables $k$ for the momentum operators $p$. The zero spectral flow for the 3D Dirac equation is shown to have a counterpart in the corresponding semi-quantum model, which is described in terms of the mapping degrees (or winding numbers) of mappings to be defined through the projection operator onto each of eigenspaces for the semi-quantum Hamiltonian. To each projection operator, there are assigned two mappings which have the mapping degrees of opposite sign. Each of the mapping degree changes the sign as the parameter passes the critical value (zero), but the net change, the sum of variation in respective mapping degrees, is zero. The zero spectral flow and the zero net change in mapping degrees are in keeping with the particle-hole symmetry of the quantum and semi-quantum Hamiltonians. Thus, the bulk-edge correspondence proves to hold in the present setting.

This paper is organized as follows: In Sec. 2, the Dirac Hamiltonian (3) and the corresponding semi-quantum Hamiltonian are characterized from the viewpoint of the time-reversal and the chiral symmetries. Section 3 is concerned with the full quantum model. In the beginning of this section, a brief review is made of the total angular momentum operators together with the associated spinor spherical harmonics on $S^2$. After the 3D Dirac Hamiltonian is described in spherical polar coordinates, a boundary operator is introduced on the two-sphere of radius $R$. Then, feasible solutions to the Dirac equation are obtained without referring to the boundary condition, which is the first step toward solutions to the boundary value problem. Depending on ranges of the parameter, the feasible solutions are classified into three classes. After the APS and the chiral bag boundary conditions are specified, eigenvalues for the 3D Dirac equation with respective boundary conditions are found together with associated eigenstates, which are classified into bulk states, edge states, and zero modes or critical states, where the radial functions for bulk and edge states are described in terms of Bessel functions and modified Bessel functions, respectively, and zero modes or critical states take the form of solid harmonics. Discrete symmetry (or pseudo-symmetry) can explain the pattern of eigenvalues as functions of the parameter $\mu$. In the last subsection of this section, the $R$-dependence of the bulk-state eigenvalues is discussed and then it is shown that the semi-quantum Hamiltonian can be viewed as a bulk Hamiltonian in the limit as $R \to \infty$. In Sec. 4, the corresponding semi-quantum Hamiltonian is studied. Two mappings $\mathbb{R}^3 \to S^3$ are defined through the projection operators onto the eigenspaces. A jump in the mapping degree against the parameter is shown to have a topological meaning. Sec. 5 presents an answer to the aforementioned question as to the correspondence between band rearrangement and topological change or the bulk-edge correspondence. In Sec. 6, remarks on further study and related fields to the present study are mentioned. Appendix A contains cal-
calculations for the derivation of spherical spinor harmonics and for the description of the Hamiltonian in the polar spherical coordinates.

2 Dirac Hamiltonians with discrete symmetry

In the momentum representation, the momentum operators \( p \) are replaced by the classical variables \( k \), and then the Dirac Hamiltonian (3) is brought into

\[
K_\mu(k) = \begin{pmatrix} \mu \mathbb{1} & -ik \cdot \sigma \\ ik \cdot \sigma & -\mu \mathbb{1} \end{pmatrix}, \quad k \in \mathbb{R}^3,
\]

which we call a semi-quantum Dirac Hamiltonian. In this section, we characterize the Hamiltonian (4) after the classification scheme for Hermitian matrices by means of discrete symmetries such as time-reversal, particle-hole, and chiral symmetries \([3, 26, 64]\). Remarks on the so-called AZ classification will be made in the last section, as far as the present Hamiltonian is concerned.

According to \([47, 45]\), the introduction of time-reversal symmetry along with the spin degrees of freedom for spin-\( \frac{1}{2} \) converts a two-level Hamiltonian acting on \( \mathbb{C}^2 \) into a four-level Hamiltonian acting on \( \mathbb{C}^2 \otimes \mathbb{C}^2 \), which we denote by \( \mathcal{H} \). We now require that this Hamiltonian admits the time-reversal and the chiral (or sublattice) symmetries by imposing the constraints,

\[
(\mathbb{1} \otimes i\sigma_2) \overline{\mathcal{H}}(\mathbb{1} \otimes (-i\sigma_2)) = \mathcal{H}, \tag{5a}
\]

\[
(\sigma_1 \otimes \mathbb{1}) \mathcal{H}(\sigma_1 \otimes \mathbb{1}) = -\mathcal{H}, \tag{5b}
\]

respectively, where the overline on \( \mathcal{H} \) denotes the complex conjugation. The time-reversal symmetry condition (5a) renders the Hamiltonian in the form

\[
\mathcal{H} = \begin{pmatrix} c & a & b \\ a & b & \bar{a} \\ c & -\bar{b} & \bar{a} \end{pmatrix}, \quad a, b, c \in \mathbb{C}, \ d \in \mathbb{R}. \tag{6}
\]

Furthermore, the chiral symmetry condition (5b) brings the Hamiltonian (6) into

\[
\mathcal{H} = \begin{pmatrix} c & ia & b \\ -ia & c & -\bar{b} \\ -\bar{b} & ia & -c \end{pmatrix}, \quad a, c \in \mathbb{R}, \ b \in \mathbb{C}. \tag{7}
\]

We note that the Hermitian matrix of the form (6) is already found in \([47, 45]\). If we set \( b = b_2 + ib_1 \) with \( b_1, b_2 \in \mathbb{R} \) and further rewrite the parameters as

\[
b_1 = -k_1, \quad b_2 = -k_2, \quad a = -k_3, \quad c = \mu, \tag{8}
\]

then the Hamiltonian (7) is put in the form

\[
\mathcal{H}(k, \mu) = \begin{pmatrix} \mu \mathbb{1} & -ik \cdot \sigma \\ ik \cdot \sigma & -\mu \mathbb{1} \end{pmatrix}. \tag{9}
\]
According to [56], the chiral (or sublattice) symmetry is the product of the time-reversal and the particle-hole symmetries. In our present case, the product of the time-reversal and the chiral operators is given by
\[(\mathbb{1} \otimes i\sigma_2)K \cdot (\sigma_1 \otimes \mathbb{1}) = (\sigma_1 \otimes i\sigma_2)K,\]  
where \(K\) denotes the complex conjugation. This operator serves as the particle-hole symmetry, and it is the rotation group defined through \(g\sigma_kg^{-1} = \sum_j \sigma_jG_{jk}\). This shows that the \(SU(2)\) action is accompanied with the transform \(k \mapsto Gk\) but the \(\mu\) is left invariant. For this reason, we can interpret \(k\) and \(\mu\) as dynamical variables and a control parameter, respectively. With this in mind, we denote \(\mathcal{H}(k, \mu)\) by \(K_\mu(k)\), which is exactly the same as (4). Then, Eq. (12) means that the Hamiltonian \(K_\mu(k)\) defined on \(\mathbb{R}^3\) is equivariant with respect to the \(SU(2)\) action. In a summary, we list the conditions that the \(K_\mu(k)\) satisfies for the time-reversal, the particle-hole, and the chiral symmetries, in this order,
\[(\mathbb{1} \otimes g)\mathcal{H}(k, \mu)(\mathbb{1} \otimes g^{-1}) = \mathcal{H}(Gk, \mu), \quad g \in SU(2),\]  
where \(G\) is the rotation group defined through \(g\sigma_kg^{-1} = \sum_j \sigma_jG_{jk}\). This shows that the \(SU(2)\) action is accompanied with the transform \(k \mapsto Gk\) but the \(\mu\) is left invariant. For this reason, we can interpret \(k\) and \(\mu\) as dynamical variables and a control parameter, respectively. With this in mind, we denote \(\mathcal{H}(k, \mu)\) by \(K_\mu(k)\), which is exactly the same as (4). Then, Eq. (12) means that the Hamiltonian \(K_\mu(k)\) defined on \(\mathbb{R}^3\) is equivariant with respect to the \(SU(2)\) action. In a summary, we list the conditions that the \(K_\mu(k)\) satisfies for the time-reversal, the particle-hole, and the chiral symmetries, in this order,
\[(\mathbb{1} \otimes i\sigma_2)K_\mu(k)(\mathbb{1} \otimes (-i\sigma_2)) = K_\mu(k),\]  
where \(G\) is the rotation group defined through \(g\sigma_kg^{-1} = \sum_j \sigma_jG_{jk}\) and \(G\) is left invariant. For this reason, we can interpret \(k\) and \(\mu\) as dynamical variables and a control parameter, respectively. With this in mind, we denote \(\mathcal{H}(k, \mu)\) by \(K_\mu(k)\), which is exactly the same as (4). Then, Eq. (12) means that the Hamiltonian \(K_\mu(k)\) defined on \(\mathbb{R}^3\) is equivariant with respect to the \(SU(2)\) action. In a summary, we list the conditions that the \(K_\mu(k)\) satisfies for the time-reversal, the particle-hole, and the chiral symmetries, in this order,
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where \(G\) is the rotation group defined through \(g\sigma_kg^{-1} = \sum_j \sigma_jG_{jk}\). This shows that the \(SU(2)\) action is accompanied with the transform \(k \mapsto Gk\) but the \(\mu\) is left invariant. For this reason, we can interpret \(k\) and \(\mu\) as dynamical variables and a control parameter, respectively. With this in mind, we denote \(\mathcal{H}(k, \mu)\) by \(K_\mu(k)\), which is exactly the same as (4). Then, Eq. (12) means that the Hamiltonian \(K_\mu(k)\) defined on \(\mathbb{R}^3\) is equivariant with respect to the \(SU(2)\) action. In a summary, we list the conditions that the \(K_\mu(k)\) satisfies for the time-reversal, the particle-hole, and the chiral symmetries, in this order,
Then, by the operation with $\sigma_3 \otimes 1$ for Eqs. (13) and (14) and without the operation for Eq. (15) and further by replacing $k$ by $p$, we find that the Dirac Hamiltonian $H_\mu(p)$ satisfies, respectively, the equations for the time-reversal, the particle-hole, and the chiral symmetries,

\[
\begin{align*}
(\sigma_3 \otimes i\sigma_2)H_\mu(p)(\sigma_3 \otimes (-i\sigma_2)) &= H_\mu(p), \\
(\sigma_2 \otimes \sigma_2)H_\mu(p)(\sigma_2 \otimes \sigma_2) &= -H_\mu(p), \\
(\sigma_1 \otimes 1)H_\mu(p)(\sigma_1 \otimes 1) &= -H_\mu(p).
\end{align*}
\]

(17)  (18)  (19)

In closing this section, we have to mention the parity. For a four-component spinor defined on $\mathbb{R}^3$, the parity transformation is defined to be $\Phi(x) \mapsto \gamma_0 \Phi(-x)$, $x \in \mathbb{R}^3$, where $\gamma_0$ is given in (2) and expressed also as $\gamma_0 = \sigma_3 \otimes 1$. As is well known, the Dirac Hamiltonian $H_\mu$ is parity invariant and transforms according to

\[
(\sigma_3 \otimes 1)H_\mu(p)(\sigma_3 \otimes 1) = H_\mu(-p).
\]

(20)

3 Full quantum Dirac models

This section, broken up into several subsections, deals with the eigenvalue problem for the Dirac operator (3) on the ball of radius $R$ under both the APS and the chiral bag boundary conditions.

3.1 A review of the total angular momentum operators

In order to solve the Dirac equation by the use of rotational symmetry, we need to review the total angular momentum operators and the spinor spherical harmonics on $S^2$.

3.1.1 The $SU(2)$ symmetry

As is already adopted in (12), the $SU(2)$ action on $\mathbb{C}^4$ is expressed by the matrix

\[
D(g) := 1 \otimes g = \begin{pmatrix} g & \ 0 \\ 0 & g \end{pmatrix}, \quad g \in SU(2).
\]

(21)

Let $\Phi$ be a four-component spinor defined on $\mathbb{R}^3$. Then, the actions of $SU(2)$ on $\mathbb{R}^3$ and on $\mathbb{C}^4$ are related through the diagram

\[
\begin{array}{ccc}
\mathbb{R}^3 & \xrightarrow{\Phi} & \mathbb{C}^4 \\
\downarrow{\text{Ad}_g} & & \downarrow{D(g)} \\
\mathbb{R}^3 & \xrightarrow{U_g \Phi} & \mathbb{C}^4
\end{array}
\]

(22)

Here, the space $\mathbb{R}^3$ is identified with $\mathcal{H}_0(2) = \{ \sum x_k \sigma_k \}$, the set of trace-less $2 \times 2$ Hermitian matrices, and the $\text{Ad}_g$ is represented as the $SO(3)$ action such as

\[
\text{Ad}_{e^{-it\sigma_k/2}} = e^{IR(e_k)}, \quad k = 1, 2, 3.
\]

(23)
where $R(a)$ is a skew-symmetric matrix defined through $R(a)x = a \times x$, $a, x \in \mathbb{R}^3$ and where $e_k$ denote the standard basis vectors of $\mathbb{R}^3$.

The diagram (22) determines the unitary operator $U_g$ acting on spinors by

$$U_g \Phi = D(g) \Phi \circ \text{Ad}_g^{-1}. \quad (24)$$

For $e^{-it\sigma_k/2}$, the generator of the unitary operator $U_{e^{-it\sigma_k/2}}$ is denoted by $-iJ_k$ and expressed as

$$J_k = \begin{pmatrix} L_k + \frac{1}{2}\sigma_k & \frac{1}{2}\sigma_k \\ \frac{1}{2}\sigma_k & L_k + \frac{1}{2}\sigma_k \end{pmatrix}, \quad k = 1, 2, 3. \quad (25)$$

The operators $J = (J_k)$ are called the total angular momentum operators or the spin-orbital angular momentum operators, satisfying the commutation relations

$$[J_j, J_k] = i \sum \varepsilon_{jkl} J_l. \quad (26)$$

Like (12), the Dirac Hamiltonian $H_\mu(p)$ admits the $SU(2)$ symmetry

$$D(g)H_\mu(p)D(g)^{-1} = H_\mu(Gp). \quad (27)$$

For $g = e^{-it\sigma_k/2}$ and $G = e^{tR(e_k)}$, the above equation is differentiated with respect to $t$ at $t = 0$ to provide

$$\left[-\frac{i}{2} \mathbb{1} \otimes \sigma_k, H_\mu\right] = \left[i \mathbb{1} \otimes L_k, H_\mu\right], \quad k = 1, 2, 3. \quad (28)$$

which implies that the Hamiltonian and the total angular momentum operators commute,

$$[H_\mu, J_k] = 0. \quad (29)$$

It then follows that the eigenvalue problem $H_\mu \Phi = E\Phi$ reduces to subproblems on the eigenspaces of $J^2 = \sum J_k^2$ or on the representation spaces of $SU(2)$.

### 3.1.2 The representation spaces for $SU(2)$

We proceed to write out the basis states of the representation spaces for the total angular momentum operators. In view of the expression (25), we see that the representation space is decomposed into the direct sum of two spaces of two-component spinors. We now provide basis spinors of the representation spaces, viewing the operator $J = L + \frac{1}{2}\sigma$ as acting on two-spinors. On account of the Clebsch-Gordan theorem applied to the spin and the orbital angular momentum coupling, for the eigenvalues $j(j + 1)$ of $J^2$, there are two possibilities of constructing the same value of $j$,

$$j = \ell + \frac{1}{2}, \quad j = (\ell + 1) - \frac{1}{2}, \quad \ell = 0, 1, 2, \ldots. \quad (30)$$

where $\ell$ is the parameter for the representation of the orbital angular momentums and $\pm \frac{1}{2}$ are spin eigenvalues.
Basis spinors of the representation spaces for the total angular momentum are composed of spherical harmonics and basis vectors for spin matrices (see Appendix A for the construction of basis spinors). The basis spinors are given, in the case of \( j = \ell + \frac{1}{2} \), by

\[
\Phi_{m}^{j(+)} = \left( \sqrt{\frac{j+m}{2j}} Y_{j-m}^{m} \frac{1}{2}, \sqrt{\frac{j-m}{2j}} Y_{j+m}^{m} \right), \quad |m| \leq j = \ell + \frac{1}{2},
\]

and in the case of \( j = (\ell + 1) - \frac{1}{2} \) by

\[
\Phi_{m}^{j(-)} = \left( \sqrt{\frac{j-m+1}{2j+2}} Y_{j-m}^{m+\frac{1}{2}} \frac{1}{2}, \sqrt{\frac{j-m+1}{2j+2}} Y_{j+m}^{m+\frac{1}{2}} \right), \quad |m| \leq j = (\ell + 1) - \frac{1}{2},
\]

where both \( \Phi_{m}^{j(+)} \) and \( \Phi_{m}^{j(-)} \) are eigenstates of \( J_{3} \) with the eigenvalue \( m \). We refer to the two-component spinors \( \Phi_{m}^{j(+)} \) and \( \Phi_{m}^{j(-)} \) as the spin-up and the spin-down states, respectively. From (31) and (32), it turns out that the the space of four-component spinors as the representation space of the total angular momentum \( J^{2} \) with the eigenvalue \( j(j+1) \) is given by

\[
V_{j}^{(+)} \oplus V_{j}^{(-)} = \text{span}\{ \Phi_{m}^{j(+)}; |m| \leq j = \ell + \frac{1}{2} \} \oplus \text{span}\{ \Phi_{m}^{j(-)}; |m| \leq j = (\ell + 1) - \frac{1}{2} \}.
\]

In describing the four-component spinors, we may express them as

\[
\Phi_{m} = \begin{pmatrix} a \Phi_{m}^{j(+)} \\ b \Phi_{m}^{j(-)} \end{pmatrix} \quad \text{or} \quad \Psi_{m} = \begin{pmatrix} a' \Phi_{m}^{j(-)} \\ b' \Phi_{m}^{j(+)} \end{pmatrix}, \quad a, b, a', b' \in \mathbb{C}.
\]

Though these four-component spinors are related by the chiral operator \( \sigma_{1} \otimes \mathbb{1} \), we have to distinguish them. In fact, as will be seen later, the APS boundary condition is invariant under the chiral operator, but the chiral bag boundary condition is not so. A way to distinguish them is to refer to parity. By using a formula about spherical harmonics (see Appendix A), we see that the \( \Phi_{m}^{j} \) and \( \Psi_{m}^{j} \) possess opposite parity,

\[
\gamma_{0} \Phi_{m}^{j}(-r) = (-1)^{j+\frac{3}{2}} \Phi_{m}^{j}(r), \quad \gamma_{0} \Psi_{m}^{j}(-r) = (-1)^{j+\frac{3}{2}} \Psi_{m}^{j}(r), \quad |r| = 1.
\]

### 3.1.3 Some formulae

We here give some formulae in advance, which will be used in solving the Dirac equation. We first need to know how \( \Phi_{m}^{j} \) and \( \Psi_{m}^{j} \) transform under the action of the operators \( \sigma \cdot L \).

A straightforward calculation with the formula (229) given in Appendix A provides

\[
\sigma \cdot L \Phi_{m}^{j(+)} = (j - \frac{1}{2}) \Phi_{m}^{j(+)}; \\
\sigma \cdot L \Phi_{m}^{j(-)} = -(j + \frac{3}{2}) \Phi_{m}^{j(-)}.
\]
On introducing the operator

\[ P = \left( \sigma \cdot L + \mathbb{1} \right) \left( \sigma \cdot L + \mathbb{1} \right), \tag{37} \]

two types of the four-spinors given in (34) can be distinguished by the property

\[ P \Phi^j_m = (j + \frac{1}{2}) \Phi^j_m, \quad P \Psi^j_m = -(j + \frac{1}{2}) \Psi^j_m. \tag{38} \]

The operator \( P \) was introduced in [15] and shown to commute with the Hamiltonian of the form \( \alpha \cdot p + \mu \beta \). Likewise, the Hamiltonian \( H_\mu \) is shown to commute with \( P \); \( [H_\mu, P] = 0 \), so that each of the eigenvalues \( \kappa = \pm (j + \frac{1}{2}) \) serves as a quantum number.

We proceed to discuss the transformation of the basis states under the action of \( \sigma_r = \sigma \cdot r / |r| \). A straightforward calculation with the recursion formulae for the associated Legendre functions, which are given in Appendix A, provides

\[ \sigma_r \Phi^j_m^{(+)} = \Phi^j_m^{(-)}, \quad \sigma_r \Phi^j_m^{(-)} = \Phi^j_m^{(+)}. \tag{39} \]

These formulae show that the action of \( \sigma_r \) exchanges the spin-up and the spin-down states.

### 3.2 Dirac Hamiltonian in spherical polar coordinates

Because of the \( SU(2) \) symmetry, the Hamiltonian \( H_\mu \) can be expressed in terms of the polar spherical coordinates \((r, \theta, \phi)\) as

\[ H_\mu = -i \gamma_r \partial_r - \frac{i}{r} (\gamma_\theta X_\theta + \gamma_\phi X_\phi) + \mu \gamma_0, \tag{40} \]

where

\[ \partial_r = \frac{\partial}{\partial r}, \quad X_\theta = \frac{\partial}{\partial \theta}, \quad X_\phi = \frac{1}{\sin \theta} \frac{\partial}{\partial \phi}, \tag{41} \]

and where

\[ \gamma_r = \begin{pmatrix} 0 & -i \sigma_r \\ i \sigma_r & 0 \end{pmatrix}, \quad \sigma_r = \begin{pmatrix} \cos \theta & e^{-i \phi} \sin \theta \\ e^{i \phi} \sin \theta & -\cos \theta \end{pmatrix}, \tag{42a} \]

\[ \gamma_\theta = \begin{pmatrix} 0 & -i \sigma_\theta \\ i \sigma_\theta & 0 \end{pmatrix}, \quad \sigma_\theta = \begin{pmatrix} -\sin \theta & e^{-i \phi} \cos \theta \\ e^{i \phi} \cos \theta & \sin \theta \end{pmatrix}, \tag{42b} \]

\[ \gamma_\phi = \begin{pmatrix} 0 & -i \sigma_\phi \\ i \sigma_\phi & 0 \end{pmatrix}, \quad \sigma_\phi = \begin{pmatrix} 0 & -ie^{-i \phi} \\ ie^{i \phi} & 0 \end{pmatrix}. \tag{42c} \]

Furthermore, we can show that

\[ H_\mu = \gamma_r \left( -i \partial_r I + \frac{i}{r} \begin{pmatrix} \sigma \cdot L & \mu \sigma \cdot r \\ \mu \sigma \cdot r & -\sigma \cdot L \end{pmatrix} \right), \tag{43} \]

where \( I \) denotes the \( 4 \times 4 \) identity matrix (see Appendix A for the proof).
3.3 A boundary operator on the sphere

In order to pose the APS boundary condition on the sphere of radius $R$, we need a boundary operator. By restricting the $H_\mu$ to the sphere of radius $R$, we define the operator $A_\mu$. The boundary operator $B_\mu$ is then defined to be $B_\mu = i\gamma_r A_\mu$ after [4] and written out, on account of (43), as

$$B_\mu = i\gamma_r A_\mu = -\frac{1}{R} \left( \sigma \cdot L \quad \mu \sigma \cdot r \quad \sigma \cdot L \right), \quad |r| = R. \quad (44)$$

In order to see a property of $B_\mu$, we use the formula

$$B_\mu \gamma_r + \gamma_r B_\mu = \frac{2}{R} \gamma_r, \quad (45)$$

which can be verified in a straightforward manner. On account of the formula (45), we show that the gamma matrix $\gamma_r$ has the exchanging property for the ($\pm$)-eigenstates of $B_\mu$. Let $\Phi^{(+)}$ be an eigenstate of $B_\mu$ associated with a positive eigenvalue $\kappa^{(+)}$, that is, $B_\mu \Phi^{(+)} = \kappa^{(+)} \Phi^{(+)}$. Operating this equation with $\gamma_r$ and using the relation (45), we obtain

$$B_\mu \gamma_r \Phi^{(+)} = -\left( \kappa^{(+)} - \frac{2}{R} \right) \gamma_r \Phi^{(+)}. \quad (46)$$

If $\kappa^{(+)} - \frac{2}{R} > 0$, this equation implies that $\gamma_r \Phi^{(+)}$ is an eigenstate associated with a negative eigenvalue of $B_\mu$. This fact will play a key role to posing the APS boundary condition. The $B_\mu$ is in principle the same as that used in [5].

3.4 Feasible solutions to the Dirac equation

We set out to solve the Dirac equation $H_\mu \Phi = E \Phi$ in the spherical polar coordinates. The APS and the chiral bag boundary conditions will be applied in Sec. 3.8 and in Sec. 3.9, respectively, to the feasible solutions obtained in this section. On account of (43) together with $\gamma_r^2 = I$, we put the eigenvalue equation in the form

$$i\gamma_r H_\mu \Phi = iE \gamma_r \Phi. \quad (47)$$

In applying the separation of variable method, Eq. (34) shows that there are two ways to express unknown states,

$$\Phi^j_m = \begin{pmatrix} f(r) \Phi^j_m^{(+)} \\ g(r) \Phi^j_m^{(-)} \end{pmatrix}, \quad \Psi^j_m = \begin{pmatrix} f(r) \Phi^j_m^{(-)} \\ g(r) \Phi^j_m^{(+)} \end{pmatrix}, \quad (48)$$

where $f, g$ are unknown functions. Writing out Eq. (47) for $\Phi = \Phi^j_m$, the left one of the two unknown states given in (48), and using the formulae about the actions of $\sigma \cdot L$ and $\sigma_r$ on $\Phi^j_m^{(\pm)}$, $\Phi^j_m^{(-)}$ given in Sec. 3.1.3, we obtain the radial equations

$$\frac{df}{dr} - \frac{\ell}{r} f = (E + \mu) g, \quad (49a)$$

$$\frac{dg}{dr} + \frac{\ell + 2}{r} g = (-E + \mu) f. \quad (49b)$$
In a similar manner, Eq. (47) with $\Phi = \Psi^j_m$ reduces to the following radial equations
\[
\frac{df}{dr} + \frac{\ell + 2}{r}f = (E + \mu)g,
\]
\[
(50a)
\]
\[
\frac{dg}{dr} - \frac{\ell}{r}g = (-E + \mu)f.
\]
\[
(50b)
\]
We are to find solutions to respective radial equations (49) and (50). In what follows, the procedure for solving those equations is divided into three, according to $|E| < |\mu|$, $|E| > |\mu|$, and $|E| = |\mu|$, and each of cases is further broken up into two, according to whether the unknown state is of the form $\Phi^j_m$ or $\Psi^j_m$ (see (48)).

3.4.1 The case of $|E| < |\mu|$

The coupled first-order differential equations (49) for $j = \ell + \frac{1}{2}$ are put together to give rise to the uncoupled second-order differential equations
\[
\frac{d^2f}{dr^2} + \frac{2}{r} \frac{df}{dr} - \left( \mu^2 - E^2 + \frac{\ell(\ell + 1)}{r^2} \right) f = 0,
\]
\[
(51a)
\]
\[
\frac{d^2g}{dr^2} + \frac{2}{r} \frac{dg}{dr} - \left( \mu^2 - E^2 + \frac{(\ell + 1)(\ell + 2)}{r^2} \right) g = 0.
\]
\[
(51b)
\]
For $\mu^2 - E^2 > 0$, these equations are modified spherical Bessel equations. We set
\[
\varepsilon = \sqrt{\mu^2 - E^2}, \quad |E| < |\mu|.
\]
(52)

Then, solutions to (51) take the form
\[
f(r) = \frac{C_1}{\sqrt{\varepsilon r}} I_{\ell + \frac{3}{2}}(\varepsilon r), \quad g(r) = \frac{C_2}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r),
\]
(53)

where $C_1, C_2$ are constants and the $I_{\ell + \frac{3}{2}}, I_{\ell + \frac{1}{2}}$ are modified Bessel functions of the first kind, and where modified Bessel functions of the second kind have been deleted on account of the regularity of solutions at the origin $r = 0$. The constants $C_1, C_2$ are to be related through (49). By using the recursion formula for the modified spherical Bessel functions,
\[
\left( \frac{d}{dr} - \frac{\ell}{r} \right) \frac{1}{\sqrt{\varepsilon r}} I_{\ell + \frac{3}{2}}(\varepsilon r) = \frac{\varepsilon}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r),
\]
(54a)
\[
\left( \frac{d}{dr} + \frac{\ell + 2}{r} \right) \frac{1}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r) = \frac{\varepsilon}{\sqrt{\varepsilon r}} I_{\ell + \frac{3}{2}}(\varepsilon r),
\]
(54b)

we find that
\[
\frac{C_1}{E + \mu} = \frac{C_2}{\sqrt{\mu^2 - E^2}}.
\]
(55)

Since the region defined by $\mu^2 - E^2 > 0$ in the $(E, \mu)$-space consists of two connected components distinguished by the sign of $\mu$ (see Fig. 1), this relation leads to
\[
\frac{C_1}{\sqrt{\mu + E}} = \frac{C_2}{\sqrt{\mu - E}} \quad \text{for} \quad \mu > 0,
\]
(56a)
\[
\frac{C_1}{-\sqrt{|\mu + E|}} = \frac{C_2}{\sqrt{|\mu - E|}} \quad \text{for} \quad \mu < 0.
\]
(56b)
It turns out that solutions to the Dirac equation for \( \Phi^j_m \) take the form

\[
\Phi^j_m = c \left( \frac{\sqrt{\mu + E}}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r) \Phi^{j(+)}_m \right) \quad \text{for } \mu > 0, \tag{57a}
\]

\[
\Phi^j_m = c' \left( \frac{\sqrt{\mu - E}}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r) \Phi^{j(-)}_m \right) \quad \text{for } \mu < 0. \tag{57b}
\]

We proceed to (50). Carrying out the same procedure, we eventually find that solutions to the Dirac equation for \( \Psi^j_m \) take the form

\[
\Psi^j_m = c \left( \frac{\sqrt{|\mu + E|}}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r) \Phi^{j(+)}_m \right) \quad \text{for } \mu > 0, \tag{58a}
\]

\[
\Psi^j_m = c' \left( \frac{\sqrt{|\mu - E|}}{\sqrt{\varepsilon r}} I_{\ell + \frac{1}{2}}(\varepsilon r) \Phi^{j(-)}_m \right) \quad \text{for } \mu < 0. \tag{58b}
\]

3.4.2 The case of \( |E| > |\mu| \)

The coupled first-order differential equations (49) for \( j = \ell + \frac{1}{2} \) are put together to provide the uncoupled second-order differential equations

\[
\frac{d^2 f}{dr^2} + 2 \frac{df}{dr} + \left( E^2 - \mu^2 - \frac{\ell(\ell + 1)}{r^2} \right) f = 0, \tag{59a}
\]

\[
\frac{d^2 g}{dr^2} + 2 \frac{dg}{dr} + \left( E^2 - \mu^2 - \frac{(\ell + 1)(\ell + 2)}{r^2} \right) g = 0. \tag{59b}
\]

For \( E^2 - \mu^2 > 0 \), these equations are spherical Bessel equations. On introducing the parameter

\[
\beta = \sqrt{E^2 - \mu^2}, \quad |E| > |\mu|, \tag{60}
\]

solutions to (59) are put in the form

\[
f(r) = \frac{C_1}{\sqrt{\varepsilon r}} J_{\ell + \frac{1}{2}}(\beta r), \quad g(r) = \frac{C_2}{\sqrt{\varepsilon r}} J_{\ell + \frac{1}{2}}(\beta r), \tag{61}
\]

where \( C_1, C_2 \) are constants and the \( J_{\ell + \frac{1}{2}} \) are Bessel functions, and where Neumann functions have been deleted on account of the regularity of solutions at the origin \( r = 0 \). The constants \( C_1, C_2 \) are related through (49). By using the recursion formula for the spherical Bessel functions,

\[
\left( \frac{d}{dr} + \frac{\ell + 2}{r} \right) \frac{1}{\sqrt{\beta r}} J_{\ell + \frac{1}{2}}(\beta r) = \frac{\beta}{\sqrt{\beta r}} J_{\ell + \frac{1}{2}}(\beta r), \tag{62a}
\]

\[
\left( \frac{d}{dr} - \frac{\ell}{r} \right) \frac{1}{\sqrt{\beta r}} J_{\ell + \frac{1}{2}}(\beta r) = -\frac{\beta}{\sqrt{\beta r}} J_{\ell + \frac{1}{2}}(\beta r). \tag{62b}
\]

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we find from (49) that
\[ \frac{C_1}{E + \mu} = - \frac{C_2}{\sqrt{E^2 - \mu^2}}. \]  
(63)

Since the region defined by \( E^2 - \mu^2 > 0 \) in the \((E, \mu)\)-space is broken up into two, according to the sign of \( E \) (see Fig. 1), this relation leads to
\[ \frac{C_1}{\sqrt{E + \mu}} = - \frac{C_2}{\sqrt{E - \mu}} \quad \text{for} \quad E > 0, \]
\[ \frac{C_1}{\sqrt{|E + \mu|}} = C_2 \quad \text{for} \quad E < 0. \]
(64a) 
(64b)

It then follows that solutions to the Dirac equation for \( \Phi^j_m \) take the form
\[
\Phi^j_m = \begin{cases} 
  c \left( - \sqrt{E + \mu} J_{\ell + \frac{1}{2}}(\beta r)\Phi^j_m(+) \right) & \text{for} \quad E > 0, \\
  c' \left( \sqrt{|E + \mu|} J_{\ell + \frac{1}{2}}(\beta r)\Phi^j_m(-) \right) & \text{for} \quad E < 0.
\end{cases}
\]
(65a) 
(65b)

3.4.3 The case of \(|E| = |\mu|\)

Equations (51) and (59) are valid for \(|E| = |\mu|\) and thereby reduce to
\[
\frac{d^2 f}{dr^2} + \frac{2 df}{r dr} - \frac{\ell(\ell + 1)}{r^2} f = 0, \]
\[
\frac{d^2 g}{dr^2} + \frac{2 dg}{r dr} - \frac{(\ell + 1)(\ell + 2)}{r^2} g = 0.
\]
(67a) 
(67b)

Solving these equations with the boundary condition that \( f \) and \( g \) be bounded as \( r \to 0 \), we obtain
\[
f(r) = ar^\ell, \quad g(r) = br^{\ell+1},
\]
(68)
where \( a \) and \( b \) are constants. These constants should be related through (49). If we impose the condition that \( E = -\mu \), Eq. (49) reduces to
\[
\frac{df}{dr} - \frac{\ell}{r} f = 0, \]
\[
\frac{dg}{dr} + \frac{\ell + 2}{r} g = 2\mu f.
\]
(69a) 
(69b)
Eqs. (68) and (69) are put together to give the ratio of $a$ and $b$, and thereby the critical solution for $\Phi^j_m$ are shown to be

$$\Phi_{cr} = c \left( \frac{(2\ell+3)r^\ell \Phi^j_m^{(+)} }{2\mu r^{\ell+1} \Phi^j_m^{(-)} } \right) \quad \text{for} \quad E = -\mu,$$

(70)

where $c$ is a constant. In contrast to this, if we impose the condition that $E = \mu$, Eq. (49) reduces to

$$\frac{df}{dr} - \frac{\ell}{r} f = 2\mu g,$$

(71a)

$$\frac{dg}{dr} + \frac{\ell + 2}{r} g = 0.$$

(71b)

Eqs. (68) and (71) are put together to provides the solution

$$\Phi'_{cr} = c' \left( \begin{array}{c} r^\ell \Phi^j_m^{(+)} \\ 0 \end{array} \right) \quad \text{for} \quad E = \mu.$$

(72)

If we start with (50), then we eventually find the following critical solutions,

$$\Psi_{cr} = c \left( \begin{array}{c} 2\mu r^{\ell+1} \Phi^j_m^{(-)} \\ (2\ell+3)r^\ell \Phi^j_m^{(+)} \end{array} \right) \quad \text{for} \quad E = \mu,$$

(73)

and

$$\Psi'_{cr} = c' \left( \begin{array}{c} 0 \\ r^\ell \Phi^j_m^{(+)} \end{array} \right) \quad \text{for} \quad E = -\mu,$$

(74)

where $c$ and $c'$ are constants.

In particular, in the case of $E = \mu = 0$, the critical solutions obtained above reduce to (72) and (74), which are called zero modes.

So far we have found feasible solutions to the Dirac equation without referring to boundary conditions, which are listed in the following table:

| $|E|=|\mu|$ | $|E|>|\mu|$ | $|E|=|\mu|$ |
|---|---|---|
| $\Phi^j_m$ | (57) | (65) | (70)/(72) |
| $\Psi^j_m$ | (58) | (66) | (73)/(74) |

(75)

These solutions are assigned to each of connected domains and the boundary lines shown in Fig. 1.

### 3.5 The APS boundary condition on the sphere

To start with, we give a basic equation on which boundary conditions are set up. Let $V$ be a domain bounded by a surface $S$. The inner products for multi-component functions on $V$ and on $S$ are defined as usual to be

$$\langle \Phi, \Psi \rangle_V = \int_V \sum_{\alpha} \overline{\Phi}_\alpha \Psi_\alpha dV, \quad \langle \phi, \psi \rangle_S = \int_S \sum_{\alpha} \overline{\phi}_\alpha \psi_\alpha dS,$$

(76)
and negative eigenvalues, if \( k \) is expected to admit the same symmetry. In fact, a straightforward calculation shows that (i) \( B \) has no zero eigenvalue and (ii) the \( \gamma \cdot n \) transforms eigenstates associated with positive eigenvalues of \( B \) to those associated with negative ones, and vice versa, and if the boundary functions \( \phi = \Phi|_S, \psi = \Psi|_S \) are required to belong to the eigenspace associated with either positive or negative eigenvalues, then the right-hand side of (77) vanishes, so that the \( H_\mu \) is a symmetric operator. Furthermore, with some Sobolev conditions, the \( H_\mu \) becomes self-adjoint [30]. The operator \( B_\mu \) we have already defined in (44) is such an operator. In fact, we have shown in Eq. (46) that the \( \gamma_\nu = \gamma \cdot n \) exchanges eigenstates associated with positive and negative eigenvalues, if \( \kappa^{(+)} - \frac{2}{R} > 0 \). We will soon show that \( \gamma_\nu \) indeed exchanges eigenstates associated with positive and negative eigenvalues (see (91)).

We shall solve eigenvalue problem for \( B_\mu \) in order to describe the APS boundary condition in an explicit form. Since the initial Dirac operator \( H_\mu \) admits an \( SU(2) \) symmetry, the \( B_\mu \), which is defined by restricting the \( H_\mu \) to the sphere of radius \( R \) and by multiplying the matrix \( i\gamma_\tau \), is expected to admit the same symmetry. In fact, a straightforward calculation shows that \( B_\mu \) commutes with \( J_k \):

\[
[B_\mu, J_k] = 0. \tag{78}
\]

On account of the \( SU(2) \) symmetry of \( B_\mu \), the eigenvalue problem for \( B_\mu \) reduces to subproblems on the eigenspaces of \( J^2 \).
3.5.1 Eigenspaces of $B_\mu$ with $\mu \neq 0$

Any state associated with the eigenvalues $J_3 = m$ and $J^2 = j(j + 1)$ is put in the form given in (34). We first take the left of (34). Then, by the use of (44) together with (36) and (39), the eigenvalue equation $B_\mu \Phi^j_m = \lambda \Phi^j_m$ reduces to the matrix eigenvalue equation

$$\frac{-1}{R} \begin{pmatrix} \ell & \mu R \\ \mu R & -(\ell + 2) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}, \quad j = \ell + \frac{1}{2}.$$  \hspace{1cm} (79)

From this equation, the eigenvalues are easily found to be

$$\lambda^{(\pm)}_j = \frac{1}{R} (1 \pm \sqrt{(\ell + 1)^2 + (\mu R)^2}),$$ \hspace{1cm} (80)

and the associated eigenvectors are easily obtained, and thereby the associated eigenstates of $B_\mu$ are expressed, within constant multiples, as

$$\Phi^{(+)}_{m,j} = \begin{pmatrix} -\mu R \Phi^{(+)}_m \\ (\ell + 1 + \sqrt{\ell + 1)^2 + (\mu R)^2}) \Phi^{(-)}_m \end{pmatrix} \quad \mathrm{for} \quad \lambda^{(+)}_j = \frac{1}{R} (1 + \sqrt{(\ell + 1)^2 + (\mu R)^2}),$$ \hspace{1cm} (81a)

$$\Phi^{(-)}_{m,j} = \begin{pmatrix} -\mu R \Phi^{(+)}_m \\ (\ell + 1 - \sqrt{\ell + 1)^2 + (\mu R)^2}) \Phi^{(-)}_m \end{pmatrix} \quad \mathrm{for} \quad \lambda^{(-)}_j = \frac{1}{R} (1 - \sqrt{(\ell + 1)^2 + (\mu R)^2}).$$ \hspace{1cm} (81b)

It is to be noted that

$$\lambda^{(+)}_j > 0, \quad \lambda^{(-)}_j < 0, \quad \text{if} \quad \mu \neq 0.$$ \hspace{1cm} (82)

Though $\Phi^{(\pm)}_{m,j}$ are not normalized, they are orthogonal to each other, as is easily verified;

$$\langle \Phi^{(+)}_{m,j}, \Phi^{(-)}_{m,j} \rangle_{S^2} = 0.$$ \hspace{1cm} (83)

We proceed to treat $\Psi^j_m$, the right of Eq. (34). Then, in a similar manner to the above, the eigenvalue equation $B_\mu \Psi^j_m = \kappa \Psi^j_m$ reduces to

$$\frac{-1}{R} \begin{pmatrix} -(\ell + 2) & \mu R \\ \mu R & \ell \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix} = \kappa \begin{pmatrix} a' \\ b' \end{pmatrix}, \quad j = \ell + \frac{1}{2},$$ \hspace{1cm} (84)

from which one easily obtains the eigenvalues

$$\kappa^{(\pm)}_j = \frac{1}{R} (1 \pm \sqrt{(\ell + 1)^2 + (\mu R)^2}),$$ \hspace{1cm} (85)

and the associated eigenvectors, and thereby the associated eigenstates of $B_\mu$ are expressed as

$$\Psi^{(+)}_{m,j} = \begin{pmatrix} -\mu R \Psi^{(-)}_m \\ (-\ell + 1 + \sqrt{\ell + 1)^2 + (\mu R)^2}) \Psi^{(+)}_m \end{pmatrix} \quad \mathrm{for} \quad \kappa^{(+)}_j = \frac{1}{R} (1 + \sqrt{(\ell + 1)^2 + (\mu R)^2}),$$ \hspace{1cm} (86a)

$$\Psi^{(-)}_{m,j} = \begin{pmatrix} -\mu R \Psi^{(-)}_m \\ (-\ell + 1 - \sqrt{\ell + 1)^2 + (\mu R)^2}) \Psi^{(+)}_m \end{pmatrix} \quad \mathrm{for} \quad \kappa^{(-)}_j = \frac{1}{R} (1 - \sqrt{(\ell + 1)^2 + (\mu R)^2}),$$ \hspace{1cm} (86b)
where
\[ \kappa_j^+ > 0, \quad \kappa_j^- < 0. \] (87)

Though these eigenstates are not normalized, they are orthogonal to each other
\[ \langle \Psi_{m,j}^+, \Psi_{m,j}^- \rangle_{S^2} = 0. \] (88)

Furthermore, the four-component spinors \( \Phi_{m,j}^\pm \) and \( \Psi_{m,j}^\pm \) are mutually orthogonal;
\[ \langle \Phi_{m,j}^+, \Psi_{m,j}^\pm \rangle_{S^2} = \langle \Phi_{m,j}^-, \Psi_{m,j}^\pm \rangle_{S^2} = 0. \] (89)

So far, for \( \mu \neq 0 \), we have obtained eigenspaces of \( B_\mu \) associated with the eigenvalues \( \lambda_j^\pm \) and \( \kappa_j^\pm \),
\[ \mathcal{H}_j^+(S^2) = \text{span}\{ \Phi_{m,j}^+; |m| \leq j = \ell + \frac{1}{2} \} \quad \text{with} \quad \lambda_j^+, \] (90a)
\[ \mathcal{K}_j^+(S^2) = \text{span}\{ \Psi_{m,j}^+; |m| \leq j = \ell + \frac{1}{2} \} \quad \text{with} \quad \kappa_j^+, \] (90b)
\[ \mathcal{H}_j^-(S^2) = \text{span}\{ \Phi_{m,j}^-; |m| \leq j = \ell + \frac{1}{2} \} \quad \text{with} \quad \lambda_j^-, \] (90c)
\[ \mathcal{K}_j^-(S^2) = \text{span}\{ \Psi_{m,j}^-; |m| \leq j = \ell + \frac{1}{2} \} \quad \text{with} \quad \kappa_j^- . \] (90d)

### 3.5.2 The APS boundary condition with \( \mu \neq 0 \)

The Hilbert space of four-component spinors on the sphere \( S^2 \) is decomposed into the direct sum of the subspaces associated with positive and negative eigenvalues of \( B_\mu \). We now show that the \( (\pm) \)-eigenspaces mutually exchange under the action of \( \gamma_r \);
\[ \gamma_r \mathcal{H}_j^+(S^2) = \mathcal{H}_j^-(S^2), \quad \gamma_r \mathcal{K}_j^+(S^2) = \mathcal{K}_j^-(S^2). \] (91)

To this end, we have only to show that
\[ \gamma_r \Phi_{m,j}^+ = \text{const} \Phi_{m,j}^-, \quad \gamma_r \Psi_{m,j}^+ = \text{const} \Psi_{m,j}^-, \] (92)

and we can easily verify these equations by using (39).

Now we are in a position to explicitly describe the APS boundary condition with \( \mu \neq 0 \): According to whether feasible solutions are of the form \( \Phi_m^j \) or \( \Psi_m^j \), the APS boundary condition is given by
\[ \Phi|_{r=R} \in \mathcal{H}_j^+(S^2) \quad \text{or} \quad \Psi|_{r=R} \in \mathcal{K}_j^+(S^2), \] (93)
or by
\[ \Phi|_{r=R} \in \mathcal{H}_j^-(S^2) \quad \text{or} \quad \Psi|_{r=R} \in \mathcal{K}_j^-(S^2). \] (94)
3.5.3 Eigenspaces of $B_0$

The remaining task is to deal with the boundary condition for $\mu = 0$. The boundary operator $B_\mu$ with $\mu = 0$ takes the form

$$B_0 = -\frac{1}{R} \begin{pmatrix} \sigma \cdot L & 0 \\ 0 & \sigma \cdot L \end{pmatrix}.$$  \hspace{1cm} (95)

For a spinor given in the left of (34), we write out the eigenvalue equation $B_0 \Phi^j_m = \lambda \Phi^j_m$ with $j = \ell + \frac{1}{2}$ to obtain

$$-\frac{1}{R} \begin{pmatrix} \ell & 0 \\ 0 & -(\ell + 2) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}. \hspace{1cm} (96)$$

The eigenvalues and eigenvectors are easily obtained, and thereby the eigenvalues and the associated eigenstates of $B_0$ with $j = \ell + \frac{1}{2}$ are expressed as

$$\Phi_0^{(-)} = c \begin{pmatrix} \Phi^{(+)}_m \\ 0 \end{pmatrix} \text{ for } \lambda_+^{(-)} = -\frac{\ell}{R}; \hspace{1cm} (97a)$$

$$\Phi_0^{(+)}) = c' \begin{pmatrix} 0 \\ \Phi^{(-)}_m \end{pmatrix} \text{ for } \lambda_+^{(+)} = \frac{\ell + 2}{R}, \hspace{1cm} (97b)$$

where $\lambda_+^{(\pm)}$ are the limits of $\lambda_{\ell+\frac{1}{2}}^{(\pm)}$ as $\mu \to 0$, respectively. Comparison between (97) with (72) shows that if evaluated on the boundary, the zero mode $\Phi_{cr}'$ is an eigenstate associated with the eigenvalue $\lambda_+^{(-)}$.

For a spinor given in the right of (34), the eigenvalue equation $B_0 \Psi^j_m = \kappa \Psi^j_m$ is solved in a similar manner, and eventually the eigenstates of $B_0$ are shown to be expressed as

$$\Psi_0^{(+)} = c \begin{pmatrix} \Phi^{(-)}_m \\ 0 \end{pmatrix} \text{ for } \kappa_-^{(+)} = \frac{\ell + 2}{R}; \hspace{1cm} (98a)$$

$$\Psi_0^{(-)} = c' \begin{pmatrix} 0 \\ \Phi^{(+)}_m \end{pmatrix} \text{ for } \kappa_-^{(-)} = -\frac{\ell}{R}, \hspace{1cm} (98b)$$

where $\kappa_-^{(\pm)}$ are the limits of $\kappa_j^{(\pm)}$ as $\mu \to 0$, respectively. Comparison of (98) with (74) shows that if evaluated on the boundary, the zero mode $\Psi_{cr}'$ is an eigenstate associated with the eigenvalue $\kappa_-^{(-)}$.

3.6 The chiral bag boundary condition on the sphere

We now make a review of the chiral bag boundary condition, according to [4]. Any four-component spinor is decomposed into the sum of chiral components,

$$\Phi = \Phi_+ + \Phi_-, \hspace{1cm} \Phi_\pm := \frac{1}{2} (I \pm \gamma \cdot n) \Phi. \hspace{1cm} (99)$$

As is easily seen, these quantities satisfy

$$\gamma \cdot n \Phi_+ = \Phi_+, \hspace{1cm} \gamma \cdot n \Phi_- = -\Phi_-, \hspace{1cm} \langle \Psi_+, \Phi_- \rangle = 0, \hspace{1cm} (100)$$
where $\Psi_+$ is defined in a similar manner. Using these properties, we can put the right-hand side of (77) in the form

$$-i\langle \phi, \gamma \cdot n \psi \rangle_S = -i\langle \phi_+, \psi_+ \rangle_S + i\langle \phi_-, \psi_- \rangle_S. \quad (101)$$

If the chiral components $\psi_\pm$ of $\psi = \Psi|_S$ and $\phi_\pm$ of $\phi = \Phi|_S$ are related by

$$\psi_- = U\gamma_0\psi_+, \quad \phi_- = U\gamma_0\phi_+, \quad (102)$$

respectively, where $U$ is any unitary operator acting on spinors defined on the boundary and further commutes with $\gamma \cdot n$, then those components satisfy

$$\langle \phi_-, \psi_- \rangle_S = \langle \phi_+, \psi_+ \rangle_S, \quad (103)$$

so that the right-hand side of (101) vanishes. Eq. (102) is called the chiral bag boundary condition.

For the sake of simplicity, we may assume that the unitary operator $U$ is a local one, which is expressed as a finite order matrix acting fiberwise on spinors. A very simple unitary matrix is given by

$$U = e^{2i\arctan e^\lambda I}, \quad (104)$$

where the $\lambda$ is a real parameter. Then, the chiral bag boundary condition (102) for $\psi = \Psi|_S$ reads

$$\gamma \cdot n \psi = -ie^{\lambda\gamma_0}\gamma_0\psi. \quad (105)$$

### 3.7 Currents on the boundary

In this section, we show that the APS and the chiral bag boundary conditions adopted in the present paper involves physically reasonable consequences for currents on the boundary. As is well known, starting with the time-dependent Dirac equation in a natural unit system ($c = \hbar = 1$), one finds the continuity equation, after a straightforward calculation,

$$\frac{\partial}{\partial t} (\psi^\dagger \psi) + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\psi^\dagger \gamma_k \psi) = 0. \quad (106)$$

The quantities $\psi^\dagger \gamma_k \psi$ are interpreted as components of the current vector. In particular, the radial component of the current vector is given by

$$\psi^\dagger \gamma_r \psi. \quad (107)$$

Since we work with the time-independent states, the continuity equation reduces to $\text{div}(\psi^\dagger \gamma \psi) = 0$. Our objective is to show that $\psi^\dagger \gamma_r \psi = 0$ on the boundary under both the APS and the chiral bag boundary conditions.

We first deal with the APS boundary condition. According to [2, 4, 46], a boundary operator $B$ used for describing a boundary condition is required to anticommute with $\gamma_r = \gamma \cdot n$, i.e., $B\gamma_r + \gamma_r B = 0$, where $n$ denotes the outward unit normal to the boundary. This requirement seems to be adopted in order that the current normal to the
boundary vanishes. However, as was shown in (45), our boundary operator \( B_\mu \) does not anticommute with \( \gamma_r \). We can show that the current normal to the boundary vanishes under the APS boundary condition in spite of the non-anticommutation of \( B_\mu \) with \( \gamma_r \). We recall that the eigenstates of \( H_\mu \) evaluated on the boundary are proportional to the eigenstates of \( B_\mu \), which are given in (81) and (86). With this in mind, we work with the current of the eigenstates \( \Phi^{(\pm)}_{m,j} \) in the direction of the outward normal to the boundary.

A straightforward calculation provides

\[
\Phi^{(\pm)}_{m,j} \, \gamma_r \, \Phi^{(\pm)}_{m,j} = i \mu R \left( \ell + 1 \pm \sqrt{(\ell + 1)^2 + (\mu R)^2} \right) \left( \Phi^{(+)\dagger}_{m,j} \Phi^{(+)}_{m,j} - \Phi^{(-)\dagger}_{m,j} \Phi^{(-)}_{m,j} \right). \tag{108}
\]

By using the formulae (39), we can show that

\[
\Phi^{(-)\dagger}_{m,j} \Phi^{(-)}_{m,j} = \Phi^{(+)\dagger}_{m,j} \Phi^{(+)}_{m,j}, \tag{109}
\]

so that Eq. (108) becomes

\[
\Phi^{(\pm)}_{m,j} \, \gamma_r \, \Phi^{(\pm)}_{m,j} = 0. \tag{110}
\]

In a similar manner, we can verify that

\[
\Psi^{(\pm)\dagger}_{m,j} \, \gamma_r \, \Psi^{(\pm)}_{m,j} = 0. \tag{111}
\]

Equations (110) and (111) imply that the current normal to the boundary vanishes for any eigenstate associated with the eigenvalues \( \lambda^{(\pm)}_j \) and \( \kappa^{(\pm)}_j \), and hence vanishes for every eigenstate satisfying the APS boundary condition.

As for the chiral bag boundary condition, it is rather easy to see that the normal component of the current vector \( \psi^{\dagger} \gamma \psi \) on the boundary sphere vanishes. In fact, from (105), one can easily verify that

\[
\psi^{\dagger} (\gamma \cdot n) \psi = 0. \tag{112}
\]

### 3.8 The eigenvalues of the Dirac operator with the APS boundary condition

We are now in a position to find the eigenvalues of the Dirac operator with the APS boundary condition. As we have already obtained feasible solutions, our task is to apply the APS boundary condition to those solutions. According to the classification of feasible solutions into three classes depending on (i) \( |E| < |\mu| \), (ii) \( |E| > |\mu| \), and (iii) \( |E| = |\mu| \), we refer to the eigenstates satisfying the APS boundary condition as (i) edge states, (ii) bulk states, and (iii) zero modes, respectively. A reason for the nomenclature will be given in respective subsections.

#### 3.8.1 Edge states

As the APS boundary conditions (94) and (93) are to be imposed on feasible solutions of the form \( \Phi^{j}_{m} \) and \( \Psi^{j}_{m} \), respectively, we work with them separately. We first apply the APS boundary condition (94) to the feasible solutions (57). For \( \mu > 0 \), the boundary condition applied to (57a) is written out and arranged as

\[
\mu \sqrt{\frac{\mu + E}{\mu - E}} I_{\ell + \frac{1}{2}}(\varepsilon R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) I_{\ell + \frac{1}{2}}(\varepsilon R). \tag{113}
\]
If $E < 0$, one has, for $\ell \geq 0$,

$$0 < \mu \sqrt{\frac{\mu + E}{\mu - E}} < \mu, \quad 0 < \mu < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (114)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (113) may have a solution. If $E > 0$, one has

$$0 < \mu < \mu \sqrt{\frac{\mu + E}{\mu - E}}, \quad 0 < \mu < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (115)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (113) may have no solution for $E$. We turn to the case of $\mu < 0$. From (57b), the boundary condition is written out and arranged as

$$|\mu| \sqrt{\frac{|\mu + E|}{|\mu - E|}} I_{\ell+\frac{1}{2}}(\varepsilon R) = \left(\frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}\right) I_{\ell+\frac{3}{2}}(\varepsilon R). \quad (116)$$

For $E > 0$, one has

$$|\mu| \sqrt{\frac{|\mu + E|}{|\mu - E|}} < |\mu|, \quad |\mu| < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (117)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (116) may have a solution. Contrary to this, for $E < 0$, one has

$$0 < |\mu| < |\mu| \sqrt{\frac{|\mu + E|}{|\mu - E|}}, \quad 0 < |\mu| < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (118)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (116) may have no solution.

We proceed to apply the APS boundary condition (94) to feasible solutions given in (58). For $\mu > 0$, one obtains from (58a) the condition

$$\mu \sqrt{\frac{\mu - E}{\mu + E}} I_{\ell+\frac{1}{2}}(\varepsilon R) = \left(\frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}\right) I_{\ell+\frac{3}{2}}(\varepsilon R). \quad (119)$$

If $E < 0$, one has

$$0 < \mu < \mu \sqrt{\frac{\mu - E}{\mu + E}}, \quad 0 < \mu < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (120)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (119) may have no solution for $E$. If $E > 0$, one has

$$0 < \mu \sqrt{\frac{\mu - E}{\mu + E}} < \mu, \quad 0 < \mu < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}. \quad (121)$$

Since $I_{\ell+\frac{1}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R)$, Eq. (119) may have a solution. We turn to the case of $\mu < 0$. For (58b), the APS boundary condition (94) yields

$$|\mu| \sqrt{\frac{|\mu - E|}{|\mu + E|}} I_{\ell+\frac{1}{2}}(\varepsilon R) = \left(\frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}\right) I_{\ell+\frac{3}{2}}(\varepsilon R). \quad (122)$$
If \( E < 0 \), one has
\[
0 < |\mu| \sqrt{\frac{|\mu - E|}{|\mu + E|}} < |\mu|, \quad |\mu| < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}.
\]
(123)

Since \( I_{\ell+\frac{3}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R) \), Eq. (122) may have a solution for \( E \). On the contrary, if \( E > 0 \), one has
\[
0 < |\mu| \sqrt{\frac{|\mu - E|}{|\mu + E|}} < |\mu|, \quad |\mu| < \frac{\ell + 1}{R} + \sqrt{\left(\frac{\ell + 1}{R}\right)^2 + \mu^2}.
\]
(124)

Since \( I_{\ell+\frac{3}{2}}(\varepsilon R) > I_{\ell+\frac{3}{2}}(\varepsilon R) \), Eq. (122) may have no solution.

The functional equations obtained above to determine edge state eigenvalues are listed as follows:

| edg(−) | \( \Phi_{m}^{j} \) | \( \Psi_{m}^{j} \) |
|--------|----------------|----------------|
| \( \mu > 0 \) \( E > 0 \) | no sol. | (119) |
| \( \mu > 0 \) \( E < 0 \) | no sol. | (113) |
| \( \mu < 0 \) \( E > 0 \) | no sol. | (116) |
| \( \mu < 0 \) \( E < 0 \) | no sol. | (122) |

(125)

Here, the symbol edg(−) indicates that the boundary conditions corresponding to the eigenvalue \( \lambda_{j}^{(−)} \) and \( \kappa_{j}^{(−)} \) (see (94)) are adopted. The functional equations (113), (116), (119), and (122) can be numerically solved to give graphs of energy eigenvalues as functions of the parameter \( \mu \). For \( j = \frac{7}{2} \) and \( R = 1 \), the graphs of energy eigenvalues are given in Fig. 2, which shows that the edge state eigenvalues are responsible for band rearrangement, where the eigenstate for \( \mu = 0 \) will be discussed later. Further, the density \( \psi^{\dagger} \psi \) for each of the edge eigenstates leans to the boundary. For these reasons, the nomenclature “edge state” has been adopted.

In the rest of this subsection, we treat the APS boundary condition (93). We show that the boundary condition (93) does not provide eigenvalues for either \( \Phi_{m}^{j} \) or \( \Psi_{m}^{j} \). If \( \Phi|_{r=R} \) for (57) is required to belong to \( \mathcal{H}_{j}^{(+)}(S^{2}) \), the boundary condition is expressed as
\[
\frac{\sqrt{\mu + E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{-\mu R} = \frac{\sqrt{\mu - E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{\ell + 1 + \sqrt{(\ell + 1)^2 + (\mu R)^2}} \quad \text{for} \quad \mu > 0,
\]
(126a)
\[
\frac{\sqrt{\mu + E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{\mu R} = \frac{\sqrt{\mu - E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{\ell + 1 + \sqrt{(\ell + 1)^2 + (\mu R)^2}} \quad \text{for} \quad \mu < 0.
\]
(126b)

Since the left-hand sides of the above equations are negative, but the right-hand sides are positive, so that no solution exists for \( E \). It then turns out that the boundary condition \( \Phi|_{r=R} \in \mathcal{H}_{j}^{(+)}(S^{2}) \) is ill.

If \( \Psi|_{r=R} \) for (58) is required to belong to \( \mathcal{K}_{j}^{(+)}(S^{2}) \), the boundary condition are brought into
\[
\frac{\sqrt{\mu + E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{-\mu R} = \frac{\sqrt{\mu - E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{-(\ell + 1) + \sqrt{(\ell + 1)^2 + (\mu R)^2}} \quad \text{for} \quad \mu > 0,
\]
(127a)
\[
\frac{\sqrt{\mu + E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{\mu R} = \frac{\sqrt{\mu - E I_{\ell+\frac{3}{2}}(\varepsilon R)/\sqrt{\varepsilon R}}}{-(\ell + 1) + \sqrt{(\ell + 1)^2 + (\mu R)^2}} \quad \text{for} \quad \mu < 0.
\]
(127b)
Figure 2: The eigenvalues for edge states with \( j = \frac{7}{2} \) are plotted against the parameter \( \mu \). As is seen from (125), the graphs going from the upper left downward to the lower right and from the lower left upward to the upper right are associated with the eigenstates of the form \( \Phi^j_m \) and \( \Psi^j_m \), respectively, where \( \Phi^j_m \) and \( \Psi^j_m \) are associated with a positive and a negative eigenvalues of \( P \), respectively.

Since the left-hand sides of the above two equations are negative but the right-hand sides are positive, the boundary condition \( \Psi|_{r=R} \in \mathcal{K}^{(+)j}(S^2) \) is ill too.

### 3.8.2 Bulk states

In a similar manner to the manipulation of edge states, we apply the APS boundary conditions (94) and (93) to feasible solutions (65) and (66) separately. We first treat the APS boundary condition (94) corresponding to \( \lambda_j^{(-)} \). From (65) and (81b), the APS boundary condition reads

\[
-\mu \sqrt{\frac{E + \mu}{E - \mu}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E > 0, \tag{128a}
\]

\[
\mu \sqrt{\frac{|E + \mu|}{|E - \mu|}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E < 0. \tag{128b}
\]

We turn to the APS boundary condition (94) corresponding to \( \kappa_j^{(-)} \). From (66) and (86b), the APS boundary condition is put in the form

\[
\mu \sqrt{\frac{E - \mu}{E + \mu}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E > 0, \tag{129a}
\]

\[
-\mu \sqrt{\frac{|E - \mu|}{|E + \mu|}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E < 0. \tag{129b}
\]
The functional equations obtained so far to determine eigenvalues for bulk states are listed as follows:

\[
\begin{array}{c|c|c}
\text{reg(–)} & \Phi_j^m & \Psi_j^m \\
E > 0 & (128a) & (129a) \\
E < 0 & (128b) & (129b)
\end{array}
\]

Here the symbol \text{reg(–)} indicates that the boundary conditions corresponding to \lambda_j^{(–)} and \kappa_j^{(–)} are adopted. Equations (128a), (128b), (129a), and (129b) are numerically solved to give eigenvalues as functions of the parameter \mu, which form bands, as is shown in Fig. 3. It is here to be noted that there are two states with the same quantum number \(j\), which are distinguished by using the operator \(P\) (see (38)).

![Figure 3](image_url)

**Figure 3:** For \(j = \frac{7}{2}\) and \(R = 1\), the eigenvalues for bulk states under the boundary conditions \(\Phi|_R \in \mathcal{H}_j^{(–)}(S^2)\) (left panel) and \(\Psi|_R \in \mathcal{K}_j^{(–)}(S^2)\) (right panel) are plotted against the parameter \(\mu\). If reflected with respect to the horizontal axis \(E = 0\), the graph in the left panel is transformed into the graph in the right panel, which is a consequence of the chiral symmetry of the present eigenvalue problem.

We proceed to the APS boundary condition (93), which requires that the boundary values belong to the eigenstates associated with \(\lambda_j^{(+)}\) or \(\kappa_j^{(+)}\). If \(\Phi|_{r=R}\) is required to belong to the eigenspace associated with the eigenvalue \(\lambda_j^{(+)}\), then from (65) and (81a), the boundary condition is expressed and arranged as

\[
\mu \sqrt{\frac{E - \mu}{E + \mu}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E > 0, \quad (131a)
\]

\[
-\mu \sqrt{\frac{|E - \mu|}{E + \mu}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for } E < 0. \quad (131b)
\]

If \(\Psi|_{r=R}\) is required to belong to the eigenspace associated with \(\kappa_j^{(+)}\), from (66) and (86a),
the boundary condition for $E > 0$ reads

$$-\mu \sqrt{\frac{E + \mu}{E - \mu}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell + \frac{1}{2}}(\beta R) \quad \text{for} \quad E > 0, \quad (132a)$$

$$\mu \sqrt{\frac{|E + \mu|}{|E - \mu|}} J_{\ell + \frac{1}{2}}(\beta R) = \left( \frac{\ell + 1}{R} + \sqrt{\left( \frac{\ell + 1}{R} \right)^2 + \mu^2} \right) J_{\ell - \frac{1}{2}}(\beta R) \quad \text{for} \quad E < 0. \quad (132b)$$

The functional equations obtained above to determine eigenvalues for bulk states are listed as follows:

$$\begin{array}{c|c|c}
\text{reg}(+) & \Phi_{j}^{m} & \Psi_{j}^{m} \\
\hline
E > 0 & (131a) & (132a) \\
E < 0 & (131b) & (132b) \\
\end{array} \quad (133)$$

Here the symbol reg(+) indicates that the boundary conditions corresponding to $\lambda_{j}^{(+)}$ and $\kappa_{j}^{(+)}$ are adopted. Equations (131a), (131b), (132a), and (132b) are numerically solved to give eigenvalues as functions of the parameter $\mu$. Solutions to respective equations form bands, which are shown in Fig. 4.

Figure 4: The eigenvalues for bulk states under the boundary condition $\Phi|_{R} \in \mathcal{H}_{j}^{(+)}(S^{2})$ (left panel) and $\Psi|_{R} \in \mathcal{K}_{j}^{(+)}(S^{2})$ (right panel) are plotted against the parameter $\mu$ with $j = \frac{7}{2}$ and $R = 1$. Like Fig. 3, this figure also exhibits the chiral symmetry of the present eigenvalue problem.

Figures 3 and 4 show that the bulk state eigenvalues form two bands, positive and negative, which have nothing to do with band rearrangement.

### 3.8.3 Zero modes

We now deal with critical solutions in the case of $|E| = |\mu|$. Among feasible solutions (70), (72), (73), and (74), the only solutions which satisfy the APS boundary conditions are (72) and (74), which are associated with the eigenvalue $E = 0$ and are called zero modes. These eigenstates correspond to eigenvalues $\lambda_{j}^{(-)}$ and $\kappa_{j}^{(-)}$ of the boundary operator with $\mu = 0$, which are limits of $\lambda_{j}^{(-)}$ and $\kappa_{j}^{(-)}$, respectively, as $\mu \to 0$. Let us be reminded of the fact that the APS boundary condition (93) never admits edge states but the APS boundary condition (94) yields edge states, which are associated with the eigenvalues
\( \lambda_j^{(-)} \) and \( \kappa_j^{(-)} \) of the boundary operator \( B_\mu \). Furthermore, both of the conditions (93) and (94) give rise to bulk states, which are away from zero modes. Figure 2 shows that zero eigenvalue is realized as limits of edge state eigenvalues as \( \mu \to 0 \), and Figs. 3 and 4 show that zero eigenvalue is never realized as limits of bulk state eigenvalue as \( \mu \to 0 \).

### 3.8.4 Zero modes as transient states

We show that the edge eigenstate indeed approaches the zero mode as \( E(\mu) \to 0 \) along with \( \mu \to 0 \). To this end, we introduce the power series \( I_\nu^P(z) \) through

\[
I_\nu(z) = \left( \frac{z}{2} \right)^\nu I_\nu^P(z), \quad I_\nu^P(z) = \sum_{n=0}^{\infty} \frac{1}{n!(\nu + n + 1)} \left( \frac{z}{2} \right)^{2n}.
\]

For \( \mu > 0 \), we take the edge eigenstate (57a) with \( E = E(\mu) \) determined by (113). By using the symbols \( I_{\ell+\frac{1}{2}}^P \) and \( I_{\ell+\frac{3}{2}}^P \), we rewrite (57a) within a constant factor as

\[
\begin{pmatrix}
\frac{\sqrt{\mu + E}}{\sqrt{\epsilon r}} I_{\ell+\frac{1}{2}}^P (\epsilon r) \Phi_m^{j(+)} \\
\frac{\sqrt{\mu - E}}{\sqrt{\epsilon r}} I_{\ell+\frac{3}{2}}^P (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix} = \frac{\epsilon \sqrt{\mu + E}}{2^{\ell+\frac{1}{2}}} \begin{pmatrix}
r^{\ell} I_{\ell+\frac{1}{2}}^P (\epsilon r) \Phi_m^{j(+)} \\
r^{\ell} I_{\ell+\frac{3}{2}}^P (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix}.
\]

Deleting the scalar factor \( \epsilon \sqrt{\mu + E}/2^{\ell+\frac{1}{2}} \), which vanishes as \( E(\mu) \to 0 \) along with \( \mu \to 0 \), we introduce an edge eigenstate

\[
\tilde{\Phi}_{\text{edg}}^{(\pm)} = \begin{pmatrix}
r^{\ell} I_{\ell+\frac{1}{2}}^P (\epsilon r) \Phi_m^{j(+)} \\
\mu - E, r^{\ell+1} I_{\ell+\frac{3}{2}}^P (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix}
\]

which remains to be associated with the same eigenvalue \( E(\mu) \). Letting \( \mu \to 0 \) and \( E(\mu) \to 0 \), we obtain the limit

\[
\tilde{\Phi}_{\text{edg}}^{(\pm)} \to \frac{1}{\Gamma(\ell + \frac{3}{2})} \begin{pmatrix}
r^{\ell} \Phi_m^{j(+)} \\
0
\end{pmatrix},
\]

which is a zero mode (see (72)). We take (57b) in turn, where \( E = E(\mu) \) is determined by (116). Rewriting (57b) as

\[
\begin{pmatrix}
-\frac{\sqrt{|\mu + E|}}{\sqrt{\epsilon r}} I_{\ell+\frac{1}{2}} (\epsilon r) \Phi_m^{j(+)} \\
\frac{\sqrt{|\mu - E|}}{\sqrt{\epsilon r}} I_{\ell+\frac{3}{2}} (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix} = \frac{\epsilon \sqrt{|\mu + E|}}{2^{\ell+\frac{1}{2}}} \begin{pmatrix}
r^{\ell} I_{\ell+\frac{1}{2}}^P (\epsilon r) \Phi_m^{j(+)} \\
-\frac{\mu - E}{2} r^{\ell+1} I_{\ell+\frac{3}{2}}^P (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix},
\]

we introduce

\[
\tilde{\Phi}_{\text{edg}}^{(-)} = \begin{pmatrix}
r^{\ell} I_{\ell+\frac{1}{2}}^P (\epsilon r) \Phi_m^{j(+)} \\
-\frac{\mu - E}{2} r^{\ell+1} I_{\ell+\frac{3}{2}}^P (\epsilon r) \Phi_m^{j(-)}
\end{pmatrix}
\]

for \( \mu < 0 \).

Letting \( E(\mu) \to 0 \) together with \( \mu \to 0 \), we obtain the limit

\[
\tilde{\Phi}_{\text{edg}}^{(-)} \to \frac{1}{\Gamma(\ell + \frac{3}{2})} \begin{pmatrix}
r^{\ell} \Phi_m^{j(+)} \\
0
\end{pmatrix},
\]

which is a zero mode (see (72)).
the same limit as (137). Equations (137) and (140) are put together to show that the 
\( \mu \)-dependent edge states \( \tilde{\Phi}_{\text{edg}}^{-} \) and \( \tilde{\Phi}_{\text{edg}}^{+} \) are continuously connected together through a 
zero mode at \( \mu = 0 \).

Starting with (58a), we introduce
\[
\tilde{\Psi}_{\text{edg}}^{(+)} = \left( \frac{\mu + E}{2} r^{\ell+1} I_{\ell+1}^{P} (\varepsilon r) \Phi_{m}^{j(-)} \right) \left( r^{\ell} I_{\ell+\frac{1}{2}}^{P} (\varepsilon r) \Phi_{m}^{j(+)\ell} \right) \text{ for } \mu > 0,
\]
and let \( E(\mu) \to 0 \) along with \( \mu \to 0 \) to get the limit
\[
\tilde{\Psi}_{\text{edg}}^{(+)} \to \frac{1}{\Gamma(\ell + \frac{3}{2})} \left( 0 \right) r^{\ell} \Phi_{m}^{j(+)} ,
\]
which is a zero mode (see (74)). Starting with (58b) in turn, we introduce
\[
\tilde{\Psi}_{\text{edg}}^{(-)} = \left( -\frac{|\mu + E|}{2} r^{\ell+1} I_{\ell+1}^{P} (\varepsilon r) \Phi_{m}^{j(-)} \right) \left( r^{\ell} I_{\ell+\frac{1}{2}}^{P} (\varepsilon r) \Phi_{m}^{j(+)\ell} \right) \text{ for } \mu < 0.
\]
Letting \( E(\mu) \to 0 \) together with \( \mu \to 0 \), we obtain the limit
\[
\tilde{\Psi}_{\text{edg}}^{(-)} \to \frac{1}{\Gamma(\ell + \frac{3}{2})} \left( 0 \right) r^{\ell} \Phi_{m}^{j(+)} ,
\]
the same limit as (142). Put together, Eqs. (142) and (144) show that the \( \mu \)-dependent 
edge states \( \tilde{\Psi}_{\text{edg}}^{-} \) and \( \tilde{\Psi}_{\text{edg}}^{+} \) are continuously connected together through a zero mode at 
\( \mu = 0 \).

3.9 The eigenvalues of the Dirac operator with the chiral bag 
boundary condition

We treat the chiral bag boundary condition (105) on the sphere of radius \( R \). On setting 
\( \gamma_{r} = \gamma \cdot n \), the condition reads
\[
\psi = -i\gamma_{r} e^{\lambda \gamma_{0} \gamma_{0}} \psi .
\]
We apply this condition to the feasible solutions in each of the cases (i) \( |E| < |\mu| \), (ii) \( |E| > |\mu| \), (iii) \( |E| = |\mu| \), in a similar manner to the APS boundary condition.

3.9.1 Edge states

For feasible solutions (57), the boundary condition (145) is written out and arranged for 
\( \mu > 0 \) as
\[
\sqrt{\frac{\mu + E}{\mu - E}} I_{\ell+\frac{1}{2}}^{P} (\varepsilon R) = e^{-\lambda} I_{\ell+\frac{3}{2}}^{P} (\varepsilon R) .
\]
where \( \varepsilon = \sqrt{\mu^2 - E^2} \). If \( \lambda > 0 \), one obtains \( I_{\ell+\frac{1}{2}}^{P} (\varepsilon R) > e^{-\lambda} I_{\ell+\frac{3}{2}}^{P} (\varepsilon R) \) from the fact that 
\( I_{\ell+\frac{1}{2}}^{P} (\varepsilon R) > I_{\ell+\frac{3}{2}}^{P} (\varepsilon R) \). Since \( \frac{\mu + E}{\mu - E} > 1 \) for \( E > 0 \) with \( \mu > E \), Eq. (146) implies that there
are no solution for $E > 0$. If $E < 0$, Eq. (146) may have a solution. For $\mu < 0$, the boundary condition (145) applied to (57) yields

$$-\sqrt{\frac{|\mu + E|}{|\mu - E|}} I_{\ell + \frac{1}{2}}(\varepsilon R) = e^{-\lambda} I_{\ell + \frac{1}{2}}(\varepsilon R).$$  \hspace{1cm} (147)$$

Though the left-hand side is negative, the right-hand side is positive, so that this equation has no solution.

We proceed to the feasible solutions (58). For $\mu > 0$, the boundary condition (145) brings about

$$\sqrt{\frac{\mu + E}{\mu - E}} I_{\ell + \frac{1}{2}}(\varepsilon R) = e^{-\lambda} I_{\ell + \frac{1}{2}}(\varepsilon R).$$  \hspace{1cm} (148)$$

Since $I_{\ell + \frac{1}{2}}(\varepsilon R) < I_{\ell - \frac{1}{2}}(\varepsilon R)$, this equation may have a solution for $E > 0$ with $\lambda > 0$ fixed, and has no solution for $E < 0$, if $|E|$ is relatively large within the restriction $|E| < |\mu|$. For $\mu < 0$, the boundary condition (145) gives rise to

$$-\sqrt{\frac{|\mu + E|}{|\mu - E|}} I_{\ell + \frac{1}{2}}(\varepsilon R) = e^{-\lambda} I_{\ell + \frac{1}{2}}(\varepsilon R).$$  \hspace{1cm} (149)$$

The left-hand side of this equation is negative but the right-hand side positive, and hence the above equation has no solution.

Among four equations obtained above, only two equations, Eqs. (146) and (148), may have solutions, which can be numerically solved to give eigenvalues as functions of the parameter $\mu$. Examples will be given later together with examples of eigenvalues for bulk states.

### 3.9.2 Bulk states

We apply the chiral bag boundary condition to the feasible solutions (65). The boundary condition (145) provides

- \hspace{1cm} (150a)$$

$$-\sqrt{\frac{E + \mu}{E - \mu}} J_{\ell + \frac{1}{2}}(\beta R) = e^{-\lambda} J_{\ell + \frac{1}{2}}(\beta R) \hspace{1cm} \text{for} \hspace{1cm} E > 0,$$

- \hspace{1cm} (150b)$$

$$\sqrt{\frac{|E + \mu|}{|E - \mu|}} J_{\ell + \frac{1}{2}}(\beta R) = e^{-\lambda} J_{\ell + \frac{1}{2}}(\beta R) \hspace{1cm} \text{for} \hspace{1cm} E < 0.$$

Applying the chiral bag boundary condition to the feasible solutions (66), we find the functional equations for $E > 0$ and for $E < 0$,

- \hspace{1cm} (151a)$$

$$\sqrt{\frac{E + \mu}{E - \mu}} J_{\ell + \frac{1}{2}}(\beta R) = e^{-\lambda} J_{\ell + \frac{1}{2}}(\beta R) \hspace{1cm} \text{for} \hspace{1cm} E > 0,$$

- \hspace{1cm} (151b)$$

$$-\sqrt{\frac{|E + \mu|}{|E - \mu|}} J_{\ell + \frac{1}{2}}(\beta R) = e^{-\lambda} J_{\ell + \frac{1}{2}}(\beta R) \hspace{1cm} \text{for} \hspace{1cm} E < 0.$$
All functional equations obtained in Sec. 3.9.2 can be numerically solved. Examples are given in Fig. 5. A characteristic of this figure is that two of eigenvalues for bulk states are connected with eigenvalues for edge states, crossing the lines determined by $|E| = |\mu|$. The upper and lower eigenvalues crossing the lines $E = \mu$ and $E = -\mu$ are associated with a negative and a positive eigenvalues of $P$, respectively. The crossing points give critical eigenvalues, which will be evaluated in the following subsection.

![Figure 5: Eigenvalues against the parameter $\mu$ under the chiral bag boundary condition with $j = \frac{7}{2}, R = 10, \lambda = 0.1$ The black solid lines of X figure form the boundary of bulk and edge regions defined by $|E| > |\mu|$ and $|E| < |\mu|$, respectively. Some numerical errors are contained in graphs for the parameter values about $|\mu| = 1.5$, which are negligible.](image)

### 3.9.3 Singular states

We discuss the singular eigenstates in the case of $|E| = |\mu|$. Applying the chiral bag boundary condition (145) to the feasible solutions (70) and (73), we obtain the eigenvalues

$$E = -\mu = -\frac{(2\ell + 3)e^{\lambda}}{2R}$$  \hspace{1cm} (152)

and

$$E = \mu = \frac{(2\ell + 3)e^{-\lambda}}{2R},$$  \hspace{1cm} (153)

respectively. At the same time, Eqs. (70) and (73) prove to be respective eigenstates.

It is to be noted that since the eigenvalues given above are not reflection symmetric with respect to the $E = 0$ axis, which means that the chiral bag boundary condition does not admit the chiral symmetry, while the Hamiltonian admits the chiral symmetry. We will discuss discrete symmetries for the eigenvalue problems in Sec. 3.10.
3.9.4 Singular states as transient states

As is indicated in Fig. 5, two of bulk eigenstates are connected with edge eigenstates through the critical eigenstates. In the following, we show that this is the case. We rewrite (57) for $\mu > 0$, by employing the functions $I_{\ell + \frac{1}{2}}^r$ and $I_{\ell + \frac{3}{2}}^r$ (see (134)), as

$$\Phi_m^j = \frac{\varepsilon^\ell \sqrt{\mu + E}}{2^{\ell + \frac{1}{2}}} \left( \frac{r^\ell I_{\ell + \frac{1}{2}}^r (\varepsilon r) \Phi_m^{j(+)} }{\frac{\mu - E}{2} r^{\ell + 1} I_{\ell + \frac{3}{2}}^r (\varepsilon r) \Phi_m^{j(-)} } \right), \tag{154}$$

where $E = E(\mu)$ is determined by (146). Deleting the scalar factor $\varepsilon^\ell \sqrt{\mu + E}$, which vanishes as $E(\mu) \to -\mu$, we introduce

$$\tilde{\Phi}_{\text{edg}} = \frac{1}{2^{\ell + \frac{1}{2}}} \left( \frac{r^\ell I_{\ell + \frac{1}{2}}^r (\varepsilon r) \Phi_m^{j(+)} }{\frac{\mu - E}{2} r^{\ell + 1} I_{\ell + \frac{3}{2}}^r (\varepsilon r) \Phi_m^{j(-)} } \right), \tag{155}$$

which remains to be an edge eigenstate associated with the same eigenvalue $E(\mu)$. Letting $E(\mu) \to -\mu$ in the above equation, we obtain, as a limit,

$$\tilde{\Phi}_{\text{edg}} \to \frac{1}{2^{\ell + \frac{1}{2}}} \left( \frac{r^\ell I_{\ell + \frac{1}{2}}^r (\varepsilon r) \Phi_m^{j(+)} }{\frac{\mu - E}{2} r^{\ell + 1} I_{\ell + \frac{3}{2}}^r (\varepsilon r) \Phi_m^{j(-)} } \right) = \frac{1}{2^{\ell + \frac{1}{2}} \Gamma(\ell + \frac{5}{2})} \left( \frac{2\ell + 3}{2\mu r^{\ell + 1}} \Phi_m^{j(-)} \right) = \tilde{\Phi}_{\text{cri}}. \tag{156}$$

Within a constant factor, the right-hand side of the above equation is equal to the critical eigenstate (70) with $E(\mu)$ given in (152).

We proceed to show that a bulk eigenstate can approach a critical eigenstate as $E(\mu) \to -\mu$. To this end, we introduce the power series $J_{\nu}^P$ through

$$J_{\nu}(z) = (\frac{z}{2})^\nu J_{\nu}^P(z), \quad J_{\nu}^P(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n! \Gamma(\nu + n + 1)} (\frac{z}{2})^{2n}. \tag{157}$$

We take the bulk eigenstate (65) for $E < 0$ and rewrite it, by using $J_{\nu}^P$, as

$$\Phi_m^j = \frac{\beta^\ell \sqrt{|E + \mu|} }{2^{\ell + \frac{1}{2}}} \left( \frac{2\ell J_{\ell + \frac{1}{2}}^P (\beta r) \Phi_m^{j(+)} }{|E - \mu| r^{\ell + 1} J_{\ell + \frac{3}{2}}^P (\beta r) \Phi_m^{j(-)} } \right), \tag{158}$$

where $E = E(\mu)$ is determined by (150b). Deleting the scalar factor $\beta \sqrt{|E + \mu|}$, which vanishes as $E(\mu) \to -\mu$, in the right-hand side of the above equation, we introduce

$$\tilde{\Phi}_{\text{reg}} = \frac{1}{2^{\ell + \frac{1}{2}}} \left( \frac{2r^\ell J_{\ell + \frac{1}{2}}^P (\beta r) \Phi_m^{j(+)} }{|E - \mu| r^{\ell + 1} J_{\ell + \frac{3}{2}}^P (\beta r) \Phi_m^{j(-)} } \right), \tag{159}$$

which remains to be a bulk eigenstates. Letting $E(\mu) \to -\mu$ with $\mu > 0$ in the right-hand side of the above equation, we obtain

$$\tilde{\Phi}_{\text{reg}} \to \frac{1}{2^{\ell + \frac{1}{2}}} \left( \frac{2r^\ell J_{\ell + \frac{1}{2}}^P (\beta r) \Phi_m^{j(+)} }{2\mu r^{\ell + 1} \Phi_m^{j(-)} } \right) = \frac{1}{2^{\ell + \frac{1}{2}} \Gamma(\ell + \frac{5}{2})} \left( \frac{2\ell + 3}{2\mu r^{\ell + 1}} \Phi_m^{j(-)} \right) = \tilde{\Phi}_{\text{cri}}. \tag{160}$$
From (156) and (160), we see that the edge and the bulk eigenstates, \( \tilde{\Phi}_{\text{edg}} \) and \( \tilde{\Phi}_{\text{reg}} \), approach the same critical eigenstate \( \tilde{\Phi}_{\text{cri}} \) as \( E(\mu) \to -\mu \). Put another way, bulk and edge eigenstates, \( \tilde{\Phi}_{\text{edg}} \) and \( \tilde{\Phi}_{\text{reg}} \), can change into each other through the critical eigenstates \( \tilde{\Phi}_{\text{cri}} \) accompanying the variation in the parameter \( \mu \).

We turn to the eigenstates (58) for \( \mu > 0 \), where \( E(\mu) \) is determined by (148) and assumed to be compatible with the limiting procedure \( E(\mu) \to \mu \). Like \( \tilde{\Phi}_{\text{edg}} \), we introduce

\[
\tilde{\Psi}_{\text{edg}} = \frac{1}{2^{\ell+\frac{3}{2}}} \left( (\mu + E)r^{\ell+1}I_{\ell+\frac{3}{2}}(\varepsilon r)\Phi_j^{(\pm)} \right),
\]

and let \( E(\mu) \to \mu \) to get

\[
\tilde{\Psi}_{\text{edg}} \to \frac{1}{2^{\ell+\frac{3}{2}}} \left( \frac{2\mu r^{\ell+1}}{\Gamma(\ell+\frac{3}{2})} \Phi_m^{j(-)} \right) = \frac{1}{2^{\ell+\frac{3}{2}}} \left( \frac{2\mu r^{\ell+1} \Phi_m^{j(-)}}{2^{\ell+\frac{3}{2}} \Gamma(\ell+\frac{5}{2})} \right) = \tilde{\Psi}_{\text{cri}}, \tag{162}
\]

The right-hand side of the above equation is the same, within a constant factor, as the critical eigenstate (73) with \( E(\mu) \) determined by (153).

Like (160), a bulk eigenstates can be shown to approach the critical eigenstate \( \tilde{\Psi}_{\text{cri}} \). We take the bulk eigenstate (66) for \( E > 0 \), where \( E = E(\mu) \) is determined by (151a) and assumed to be compatible with the limiting procedure \( E(\mu) \to \mu \). Like (159), we introduce,

\[
\tilde{\Psi}_{\text{reg}} = \frac{1}{2^{\ell+\frac{3}{2}}} \left( (E + \mu)r^{\ell+1}I_{\ell+\frac{3}{2}}(\beta r)\Phi_j^{(\pm)} \right),
\]

Letting \( E(\mu) \to \mu \), we verify that

\[
\tilde{\Psi}_{\text{reg}} \to \frac{1}{2^{\ell+\frac{3}{2}}} \left( \frac{2\mu r^{\ell+1}}{\Gamma(\ell+\frac{3}{2})} \Phi_m^{j(-)} \right) = \frac{1}{2^{\ell+\frac{3}{2}}} \left( \frac{2\mu r^{\ell+1} \Phi_m^{j(-)}}{2^{\ell+\frac{3}{2}} \Gamma(\ell+\frac{5}{2})} \right) = \tilde{\Psi}_{\text{cri}}, \tag{164}
\]

which is the same limit as (162). Eqs. (162) and (164) are put together to imply that the edge and the bulk eigenstates, \( \tilde{\Psi}_{\text{edg}} \) and \( \tilde{\Psi}_{\text{reg}} \), change into each other through the critical eigenstate \( \tilde{\Psi}_{\text{cri}} \), like \( \tilde{\Phi}_{\text{edg}} \) and \( \tilde{\Phi}_{\text{reg}} \).

### 3.10 Discrete symmetries

We have already characterized in Sec. 2 the Dirac Hamiltonian (3) in terms of discrete symmetries. We now observe that discrete symmetries are realized in the pattern of eigenvalues as functions of the parameter \( \mu \) (see Figs. 2, 3, 4, and 5). To this end, we need to discuss the invariance of the APS and the chiral bag boundary conditions.

We first take up the chiral operator \( \sigma_1 \otimes \mathbb{1} \). A straightforward calculation with \( \sigma_1 \otimes \mathbb{1} \) provides

\[
\begin{align*}
(\sigma_1 \otimes \mathbb{1})H_\mu(\sigma_1 \otimes \mathbb{1}) & = -H_\mu, \\
(\sigma_1 \otimes \mathbb{1})B_\mu(\sigma_1 \otimes \mathbb{1}) & = B_\mu, \\
(\sigma_1 \otimes \mathbb{1})J_k(\sigma_1 \otimes \mathbb{1}) & = J_k, \\
(\sigma_1 \otimes \mathbb{1})P(\sigma_1 \otimes \mathbb{1}) & = -P,
\end{align*}
\]
where $H_\mu$ and $B_\mu$ are the Hamiltonian and the boundary operators, respectively, and where $J_k$ and $P$ are the total angular momentum operators of $4 \times 4$ matrix form and the operator distinguishing the spinor type $\Phi^j_m$ or $\Psi^j_m$ (see (38)). The chiral symmetry (165a) may be called an energy-reflecting symmetry, i.e., if $E$ is an energy eigenvalue, then so is $-E$. Eq. (165b) means that the APS boundary condition is chiral-invariant. Eq. (165c) implies that the total angular momentum quantum number $j$ and the eigenvalue $m$ of $J_3$ are invariant, but Eq. (165d) shows that the spinor type is inverted under the chiral transformation. It then turns out that if an eigenstate $\Phi$ is assigned by the quantum numbers $(E, j, m, \pm)$ then $(\sigma_1 \otimes 1)\Phi$ becomes an eigenstate assigned by the quantum numbers $(-E, j, m, \mp)$, where the signs + and − indicate that the eigenvalue of $P$ is positive and negative, respectively. This fact can explain the pattern symmetry of Figs. 2, 3, and 4 for the eigenvalues under the APS boundary condition: The two curves of eigenvalue functions shown in Fig. 2 are reflection symmetric with respect to the $\mu$-axis in the $(\mu, E)$-plane, if the inversion of $P$-eigenvalue is taken into account. The two panels in Fig. 3 are related by $\sigma_1 \otimes 1$: If we reflect the graph of the left panel with respect to the $\mu$-axis the resultant graph coincides with that of the right panel. The same procedure can be performed with Fig. 4 to observe the same pattern symmetry.

In contrast to this, the pattern of eigenvalues observed in Fig. 5 for the Dirac equation under the chiral bag boundary condition is quite different from the pattern under the APS boundary condition. Though the Hamiltonian admits the chiral symmetry, the pattern of energy eigenvalues does not exhibit the energy-reflection symmetry. This is because the chiral bag boundary condition is not invariant under the action of the chiral operator. In fact, if $\psi$ is subject to $\psi = -i \gamma_r e^{\lambda_0} \gamma_0 \psi$ then $(\sigma_1 \otimes 1)\psi$ is subject to

$$
(\sigma_1 \otimes 1)\psi = -i \gamma_r e^{-\lambda_0} \gamma_0 (\sigma_1 \otimes 1)\psi,
$$

where $\lambda$ has changed into $-\lambda$.

We turn to the particle-hole symmetry. We easily verify that

$$
(\sigma_2 \otimes \sigma_2) \mathbb{P}_\mu (\sigma_2 \otimes \sigma_2) = -H_\mu, \quad (167a)
$$

$$
(\sigma_2 \otimes \sigma_2) \mathbb{B}_\mu (\sigma_2 \otimes \sigma_2) = B_\mu, \quad (167b)
$$

$$
(\sigma_2 \otimes \sigma_2) \mathbb{J}_k (\sigma_2 \otimes \sigma_2) = -J_k, \quad (167c)
$$

$$
(\sigma_2 \otimes \sigma_2) \mathbb{J}^2 (\sigma_2 \otimes \sigma_2) = J^2, \quad (167d)
$$

$$
(\sigma_2 \otimes \sigma_2) \mathbb{P} (\sigma_2 \otimes \sigma_2) = -P. \quad (167e)
$$

The above equations imply that if $\Phi$ is an eigenstate associated with the quantum numbers $(E, j, m, \pm)$ under the APS boundary condition then $(\sigma_2 \otimes \sigma_2) K \Phi$ is an eigenstate associated with the quantum numbers $(-E, j, -m, \mp)$, where $K$ denotes the complex conjugation. Since the inversion $m \mapsto -m$ makes no appearance in the eigenvalue pattern, the chiral and the particle-hole symmetries make no difference in the eigenvalue pattern under the APS boundary condition, but the chiral operator is unitary while the particle-hole operator is anti-unitary.

Contrary to this, the chiral bag boundary condition is not invariant under the operator $(\sigma_2 \otimes \sigma_2) K$. In fact, we easily verify that if $\psi$ is subject to $\psi = -i \gamma_r e^{\lambda_0} \gamma_0 \psi$ then
\((\sigma_2 \otimes \sigma_2)K\psi\) is subject to
\[
(\sigma_2 \otimes \sigma_2)K\psi = i\gamma_re^{-\lambda\gamma_0\gamma_0}(\sigma_2 \otimes \sigma_2)K\psi.
\] (168)

We now deal with the time-reversal symmetry. A straightforward calculation with
\((\sigma_3 \otimes i\sigma_2)K\) provides
\[
\begin{align*}
(\sigma_3 \otimes i\sigma_2)\bar{H}_\mu(\sigma_3 \otimes (-i\sigma_2)) &= H_\mu, \\
(\sigma_3 \otimes i\sigma_2)\bar{B}_\mu(\sigma_3 \otimes (-i\sigma_2)) &= B_\mu, \\
(\sigma_3 \otimes i\sigma_2)\bar{J}_k(\sigma_3 \otimes (-i\sigma_2)) &= -J_k, \\
(\sigma_3 \otimes i\sigma_2)\bar{J}^2(\sigma_3 \otimes (-i\sigma_2)) &= J^2, \\
(\sigma_3 \otimes i\sigma_2)\bar{P}(\sigma_3 \otimes (-i\sigma_2)) &= P.
\end{align*}
\] (169)

Equations (169) mean that if \(\Phi\) is an eigenstate assigned by quantum numbers \((E, j, m, \pm)\) under the APS boundary condition then \((\sigma_3 \otimes i\sigma_2)K\Phi\) becomes an eigenstates assigned by the quantum numbers \((E, j, -m, \pm)\), where the Kramers degeneracy is realized as the inversion \(m \mapsto -m\) with \(E\) kept invariant.

Unlike the chiral and the particle-hole operators, the time-reversal operator leaves the chiral bag boundary condition invariant. In fact, one verifies that if \(\psi\) is subject to
\[
\psi = -i\gamma_re^{\lambda\gamma_0\gamma_0}\psi
\] then \((\sigma_3 \otimes i\sigma_2)K\psi\) is also subject to
\[
(\sigma_3 \otimes i\sigma_2)K\psi = -i\gamma_re^{\lambda\gamma_0\gamma_0}(\sigma_3 \otimes i\sigma_2)K\psi.
\] (170)

Hence, the Kramers degeneracy takes place for energy eigenvalues under the chiral bag boundary condition, like energy eigenvalues under the APS boundary condition.

### 3.11 Spectral flows under the APS and the chiral bag boundary conditions

While the bulk state eigenvalues have nothing to do with band rearrangement, the edge state eigenvalues are responsible for the band rearrangement under both of the APS and the chiral bag boundary conditions, as was seen in the behavior of eigenvalues against the parameter \(\mu\) (see Figs. 2 and 5). We now single out the eigenvalues responsible for the band rearrangement to draw illustrative figures (see Fig. 6).

The spectral flow for a one-parameter family of operators is defined to be the net number of eigenvalues passing through zero in the positive direction as the parameter runs [51]. For the eigenvalues under the APS boundary condition, the spectral flow is found to be \((-1) + 1 = 0\), where +1 is assigned to the the edge state eigenvalue with \(P < 0\) and \(-1\) to that with \(P > 0\), where \(P < 0\) and \(P > 0\) mean that the eigenvalue of \(P\) is negative and positive, respectively.

In the case of the chiral bag boundary condition, there exist transient eigenvalue curves which cross one of the boundary lines \(E = \pm \mu\), depending on whether the eigenvalues of \(P\) is positive or negative. In this case, the original definition of spectral flow cannot apply, since the crossing of the \(E = 0\) value has no meaning in band rearrangement. However, we can extend the notion of spectral flow by assigning \(-1\) and \(+1\) to the crossing of the
boundary lines $E = -\mu$ and $E = \mu$, respectively. Put another way, the numbers $+1$ and $-1$ are allotted to the transient eigenvalue curves associated with $P < 0$ and $P > 0$, respectively. Then, the extended spectral flow under the chiral bag boundary condition is $(-1) + 1 = 0$, the same as that under the APS boundary condition.

### 3.12 $R$-dependence of the bulk-state eigenvalues

Though the bulk-state eigenvalues have nothing to do with band rearrangement, they are under the influence of band rearrangement. To see this, we start by studying the $R$-dependence of the bulk-state eigenvalues. For the sake of simplicity, we first consider the bulk-state eigenvalues determined by (128a) with $\mu = 0$. The eigenvalues are then determined by the zeros of the Bessel function $J_{\ell + \frac{1}{2}}$. Let $\eta_n$ be the zeros of $J_{\ell + \frac{1}{2}}$, where $0 < \eta_1 < \eta_2 < \cdots$ with $\eta_n \to \infty$. Then, we obtain $\beta R = \eta_n$ with $\beta = E$, so that the eigenvalues are given by $E_n = \eta_n/R$. As is seen form the asymptotic behavior of the Bessel function,

$$J_{\nu}(x) \sim \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{2\nu + 1}{4}\pi\right),$$

(171)

the difference, $\eta_{n+1} - \eta_n$, between consecutive pair of zeros is approximately constant in $n$. Accordingly, the difference $E_{n+1} - E_n$ is approximately inversely proportional to $R$. If $\mu \neq 0$, a similar consequence will be brought about for small $\mu$. Equation (128a) for $E > 0$ with $\mu \neq 0$ shows that the solutions to this equation are obtained from the intersection points of the the graphs of the left- and the right-hand sides as functions of $E$. As is well known, there lies one and only one zero of $J_{\nu+1}$ between any two consecutive zeros of $J_{\nu}$ [60]. Since the factor $\sqrt{(E + \mu)/(E - \mu)}$ plays the role of an amplitude factor, the intersection points of the graphs of the left- and the right-hand sides of (128a) take place once and only once over the interval between any consecutive zeros of $J_{\ell + \frac{1}{2}}$. Let $\xi_n$ denote the projection of each intersection point to the axis of the independent variable,
$0 < \xi_1 < \xi_2 < \cdots$ with $\xi_n \to \infty$ as $n \to \infty$. Then, one has $\beta R = \xi_n$. The same reasoning applies to Eq. (129b) to give negative eigenvalues. It then turns out that the bulk-state eigenvalues determined by (128a) and (129b) are expressed as

$$E_n = \pm \sqrt{(\xi_n/R)^2 + \mu^2}. \tag{172}$$

The other bulk-state eigenvalues are expressed in the same manner. For $\mu$ small, $E_n > 0$ is approximated as $E_n \approx \xi_n R (1 + \frac{\mu^2 R^2}{2 \xi_n})$. If $\xi_n/R$ are sufficiently larger than $\mu$, the difference $E_{n+1} - E_n$ is approximately

$$E_{n+1} - E_n \approx \frac{\xi_{n+1} - \xi_n}{R} + \frac{\mu^2}{2} \left( \frac{R}{\xi_{n+1}} - \frac{R}{\xi_n} \right). \tag{173}$$

As is seen from the asymptotic behavior (171) and the functional equation (128a), the difference $\xi_{n+1} - \xi_n$ can be approximately estimated, from the zeros of $J_{\nu+1}(x) - J_\nu(x)$, to be nearly constant (within a vicinity of $\pi$) in $n$. Hence, $E_{n+1} - E_n$ is approximately proportional to $1/R$. A similar reasoning can apply to other defining equations for bulk-state eigenvalues under the chiral bag boundary condition.

It then turns out that if $R$, which is, physically speaking, looked on as representing the system size, is sufficiently large, then the energy levels become of high density, so that the bands of bulk-states eigenvalues are allowed to be treated in terms of classical variables. Like transition from Fourier series to Fourier integral along with the period tending to infinity, the momentum operators $-i\partial/\partial q_k$ in the Hamiltonian $H_\mu$ can be replaced by the classical momentum variables, like a consequence of the Fourier transform. Accordingly, the Hamiltonian $H_\mu$ turns into a semi-quantum Hamiltonian, which we denote by $K_\mu$ and has been given in Eq. (4). In the following section, we will study the “bulk” Hamiltonian $K_\mu$ to observe a topological change corresponding to the spectral flow attributed to the edge-state eigenvalues. As will be soon mentioned in the next section, in the present procedure the discrete variable $\xi_n/R$ may be viewed as changing into a continuous radial variable $k$ in the momentum space. However, we have to look on $k = 0$ as a singular value with respect to the procedure $R \to \infty$, and hence the singularity may correspond to the edge-state eigenvalues and be concerned with corresponding topological change.

## 4 Semi-quantum Dirac models

We are interested in a correspondence between the energy level transfer for the 3D Dirac equation studied in Sec. 3.8 and a topological change to be observed in the corresponding semi-quantum Hamiltonian. In the two-dimensional case, a similar correspondence has been already found in [40].

### 4.1 Projection operators onto eigenspaces

Now we work with the semi-quantum Hamiltonian (4) in detail. Since

$$\det(\lambda I - K_\mu) = (\lambda^2 - (\mu^2 + k^2))^2, \quad k^2 = k_1^2 + k_2^2 + k_3^2, \tag{174}$$

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the eigenvalues of $K_\mu$ are given by

$$\lambda^\pm(k) = \pm \sqrt{\mu^2 + k^2}. \quad (175)$$

Here, we note that each of $\lambda^\pm(k)$ is doubly degenerate, a consequence of the time-reversal symmetry. Further, the chiral symmetry results in the fact that $\lambda^-(k) = -\lambda^+(k)$. In addition, each of the eigenvalues $\lambda^\pm(k)$ may be viewed as a limit of the bulk-state eigenvalues (172) under the procedure in which the discrete variable $\xi_n/R$, $n = 1, 2, \ldots$, changes into the radial variable $k$ in the momentum space, as $R$ tends to infinity.

For the eigenvalue $\lambda^+(k)$, we have two expressions, “up” and “down”, of associated orthonormalized eigenvectors, which are

$$|u^+_{up}(k)\rangle_1 = \frac{1}{N^+_{up}} \begin{pmatrix} k_3 \\ k_1 + ik_2 \\ i(\lambda^+ - \mu) \\ 0 \end{pmatrix}, \quad |u^+_{up}(k)\rangle_2 = \frac{1}{N^+_{up}} \begin{pmatrix} k_1 - ik_2 \\ -k_3 \\ 0 \\ i(\lambda^+ - \mu) \end{pmatrix}, \quad (176)$$

$$|u^+_{down}(k)\rangle_1 = \frac{1}{N^+_{down}} \begin{pmatrix} -i(\lambda^+ + \mu) \\ 0 \\ k_3 \\ k_1 + ik_2 \end{pmatrix}, \quad |u^+_{down}(k)\rangle_2 = \frac{1}{N^+_{down}} \begin{pmatrix} 0 \\ -i(\lambda^+ + \mu) \\ k_1 - ik_2 \\ -k_3 \end{pmatrix}, \quad (177)$$

where

$$N^+_{up} = \sqrt{2\lambda^+ (\lambda^+ - \mu)}, \quad N^+_{down} = \sqrt{2\lambda^+ (\lambda^+ + \mu)}. \quad (178)$$

We here notice that the words “up” and “down” used in the semi-quantum model do not allude to spin. For $\mu > 0$, the eigenvectors $|u^+_{up}(k)\rangle_a$, $a = 1, 2$, are defined on $\mathbb{R}^3 - \{0\}$, but for $\mu < 0$ they are defined on the whole $\mathbb{R}^3$. In contrast with this, for $\mu > 0$, the eigenvectors $|u^+_{down}(k)\rangle_a$, $a = 1, 2$, are defined on $\mathbb{R}^3$, but for $\mu < 0$ they are defined on $\mathbb{R}^3 - \{0\}$. We call a point $k$ an exceptional point, if the eigenvector in question is not defined at the point $k$. For example, the origin $k = 0$ is an exceptional point of $|u^+_{up}(k)\rangle_a$, $a = 1, 2$, for $\mu > 0$.

The normalized eigenvectors associated with the eigenvalue $\lambda^-(k)$ are expressed, in the same manner, as

$$|u^-_{up}(k)\rangle_1 = \frac{1}{N^-_{up}} \begin{pmatrix} k_3 \\ k_1 + ik_2 \\ i(\lambda^- - \mu) \\ 0 \end{pmatrix}, \quad |u^-_{up}(k)\rangle_2 = \frac{1}{N^-_{up}} \begin{pmatrix} k_1 - ik_2 \\ -k_3 \\ 0 \\ i(\lambda^- - \mu) \end{pmatrix}, \quad (179)$$

$$|u^-_{down}(k)\rangle_1 = \frac{1}{N^-_{down}} \begin{pmatrix} -i(\lambda^- + \mu) \\ 0 \\ k_3 \\ k_1 + ik_2 \end{pmatrix}, \quad |u^-_{down}(k)\rangle_2 = \frac{1}{N^-_{down}} \begin{pmatrix} 0 \\ -i(\lambda^- + \mu) \\ k_1 - ik_2 \\ -k_3 \end{pmatrix}, \quad (180)$$

where

$$N^-_{up} = \sqrt{2\lambda^- (\lambda^- - \mu)} = \sqrt{2|\lambda^-|(|\lambda^-| + \mu)} = N^+_{down}, \quad N^-_{down} = \sqrt{2\lambda^- (\lambda^- + \mu)} = \sqrt{2|\lambda^-|(|\lambda^-| - \mu)} = N^+_{up}. \quad (181)$$
The exceptional point for $|u_{\text{up/down}}^-(k)\rangle$ can be identified in a similar manner to that for $|u_{\text{up/down}}^+(k)\rangle$. Accompanying the variation of the parameter $\mu$, the origin $k = 0$ is attached as an exceptional points to eigenvectors associated with either positive or negative eigenvalue, which is summed up as follows:

\[
\begin{array}{c|c|c|c}
   k = 0 & \mu < 0 & \mu = 0 & \mu > 0 \\
   \text{ex. pt. for } |u_{\text{up}}^+(k)\rangle & - & \text{deg. pt.} & + \\
   \text{ex. pt. for } |u_{\text{down}}^+(k)\rangle & + & \text{deg. pt.} & - \\
\end{array}
\]  (182)

The eigenvectors $|u_{\text{up}}^+(k)\rangle$ and $|u_{\text{down}}^+(k)\rangle$ are related on the intersection of respective domains through

\[
|u_{\text{down}}^+(k)\rangle = \sum |u_{\text{up}}^+(k)\rangle U_{ab}^+. 
\]  (183)

Calculating the matrix elements $\langle u_{\text{up}}^+(k)\rangle u_{\text{down}}^+(k)\rangle$, we find the explicit expression of $U^+ = (U_{ab}^+)$ as

\[
U^+ = \begin{pmatrix}
   -\frac{i k_1}{k} & -\frac{i k_1 - i k_2}{k} \\
   -\frac{i k_1 + i k_2}{k} & \frac{i k_2}{k}
\end{pmatrix} = -\frac{i}{k} k \cdot \sigma. 
\]  (184)

The transformation matrix $U^- = (U_{ab}^-)$ to be determined in a similar manner to (183) is found to be given by

\[
U^- = \begin{pmatrix}
   \frac{i k_1}{k} & \frac{i k_1 - i k_2}{k} \\
   \frac{i k_1 + i k_2}{k} & -\frac{i k_2}{k}
\end{pmatrix} = \frac{i}{k} k \cdot \sigma. 
\]  (185)

We now calculate the projection operators $P_\pm$ onto the eigenspaces associated with the eigenvalues $\lambda^\pm(k)$.

\[
P_+ = \frac{1}{2\lambda^+} \begin{pmatrix}
   (\lambda^+ + \mu) \mathbb{1} & -i k \cdot \sigma \\
   i k \cdot \sigma & (\lambda^+ - \mu) \mathbb{1}
\end{pmatrix} = \frac{1}{2\lambda^+} (\lambda^+ I + K_\mu), 
\]  (186)

\[
P_- = \frac{1}{2\lambda^-} \begin{pmatrix}
   (\lambda^- + \mu) \mathbb{1} & -i k \cdot \sigma \\
   i k \cdot \sigma & (\lambda^- - \mu) \mathbb{1}
\end{pmatrix} = \frac{1}{2\lambda^-} (\lambda^- I + K_\mu), 
\]  (187)

respectively, where $I$ denotes the $4 \times 4$ identity matrix.

### 4.2 Eigen-vector bundles

In this subsection, we denote the eigenvectors by $|u_{\text{up}}^+(k, \mu)\rangle$ etc., in order to stress their dependence on $k$ and $\mu$. We denote by $V^\pm(k, \mu)$ the eigenspaces associated with the eigenvalues $\lambda^\pm(k, \mu)$, where $\text{dim}_C V^\pm(k, \mu) = 2$ for $\mu \neq 0$. Then, the totality of the eigenspaces, $V^\pm(\mu) = \bigcup_{k \in \mathbb{R}^3} V^\pm(k, \mu)$, form respective vector bundles over $\mathbb{R}^3$ for $\mu \neq 0$, which we call the eigen-vector bundles associated with the eigenvalues. From the table (182), we see that the “up” eigenvectors $|u_{\text{up}}^+(k, \mu)\rangle$ and $|u_{\text{up}}^+(k, \mu)\rangle$ have no exceptional point at $k = 0$ for $\mu < 0$ and for $\mu > 0$, respectively. This implies that $V^+(\mu)$ and $V^-(\mu)$ are trivial vector bundles for $\mu < 0$ and for $\mu > 0$, respectively. Furthermore, the “down” eigenvectors $|u_{\text{down}}^-(k, \mu)\rangle$ and $|u_{\text{down}}^-(k, \mu)\rangle$ have no exceptional point for $\mu < 0$ and for $\mu > 0$, respectively, so that the eigen-vector bundles $V^-(\mu)$ and $V^+(\mu)$ are trivial for $\mu < 0$ and for $\mu > 0$. It then seems that the bundle structure $V^+(\mu) \oplus V^-(\mu)$ receives no topological change when the parameter passes the critical point $\mu = 0$ from
the $\mu < 0$ side to the $\mu > 0$ side. However, topological change takes place, accompanying the variation of the parameter $\mu$ passing the critical value $\mu$, as will be shown in the succeeding subsections.

A naive way to detect a change in term of topological quantity is to refer to Chern numbers assigned to the vector bundles $V^{\pm}(\mu)$. However, this way proves bad. Though one can calculate the connections $A^{\pm}$ and the curvatures $F^{\pm}$ for $V^{\pm}(\mu)$ with $\mu \neq 0$, the first Chern forms, which are defined to be $\text{tr} F^{\pm}$ within a constant factor, vanishes, since they take values in $\mathfrak{su}(2)$ as a consequence of the fact that the structure groups are $SU(2)$ (see (184) and (185)). Further, the Chern-Simon form $\text{tr}(A \wedge dA + \frac{2}{3} A \wedge A \wedge A)$ also vanishes and gives no information of topological property.

In spite of this fact, we are interested in looking for what change takes place when the parameter $\mu$ runs through $\mu = 0$. To this end, we look into the decomposition $V^{+}(k, \mu) \oplus V^{-}(k, \mu)$. Though this decomposition fails at $k = 0$ when $\mu = 0$, it may be viewed as surviving in a sense. In fact, we can verify that

$$\lim_{\mu \uparrow 0} V^{+}(0, \mu) = \text{span}_\mathbb{C}\{|e_3\rangle, |e_4\rangle\} = \lim_{\mu \downarrow 0} V^{-}(0, \mu), \quad (188a)$$

$$\lim_{\mu \uparrow 0} V^{-}(0, \mu) = \text{span}_\mathbb{C}\{|e_1\rangle, |e_2\rangle\} = \lim_{\mu \downarrow 0} V^{+}(0, \mu), \quad (188b)$$

where $\mu \uparrow 0$ and $\mu \downarrow 0$ means that $\mu$ tends to zero, taking negative and positive values, respectively, and where $|e_k\rangle, k = 1, \ldots, 4$, are the standard basis vectors with the $k$-th component one and the others zero. It then turns out that the degenerate positive (resp. negative) eigenvalue $\lambda^{+}(0, \mu) = |\mu|$ for $\mu < 0$ (resp. $\lambda^{-}(0, \mu) = -|\mu|$ for $\mu < 0$) goes down (resp. up) to degenerate negative (resp. positive) eigenvalue $\lambda^{-}(0, \mu) = -|\mu|$ for $\mu > 0$ (resp. $\lambda^{+}(0, \mu) = |\mu|$ for $\mu > 0$) through the totally degenerate zero eigenvalue at $k = 0$ as $\mu$ runs in the positive direction, passing $\mu = 0$. Put another way, two energy levels cross each other at $k = 0$, when $\mu = 0$. It is to be noted that the level crossing occurs at $k = 0$ only and no crossing at $k \neq 0$. This phenomenon is a realization of the singularity alluded to in the last sentence of Sec. 3.12 and we may expect that the level crossing gives rise to a certain topological change.

### 4.3 Introducing “Q matrices”

In order to seek for a suitable topological invariant to describe a topological change against the parameter in the semi-quantum model, we are reminded of the fact that for the semi-quantum model corresponding to the 2D Dirac equation the winding number (or a delta-Chern) associated with the $2 \times 2$ semi-quantum Hamiltonian plays a key role [39, 40]. In an analogous manner, we are to seek for a suitable winding number (or mapping degree) associated with the Hamiltonian $K_{\mu}(k)$.

According to a paper [56], a “Q matrix” is associated with a projection matrix. Let $P$ be a projection matrix of rank $m$ (different from the operator given in (37)), of which the complementary projection operator is assumed to be of rank $n$. The $Q$ matrix is defined to be

$$Q = 2P - I, \quad (189)$$
where $I$ is the identity matrix of order $m + n$. Since $P^2 = P$, $P^\dagger = P$, $\text{tr} P = m$, the $Q$ matrix satisfies

$$Q^\dagger = Q, \quad Q^2 = I, \quad \text{tr}Q = m - n.$$  

(190)

For the semi-quantum Hamiltonian $K_{\mu}$, the $Q$ matrices corresponding to the projection operators (186) and (187) are obtained as follows:

$$Q_+ = \frac{1}{\lambda^+} K_{\mu}, \quad Q_- = \frac{1}{\lambda^-} K_{\mu},$$  

(191)

respectively, where $m = n = 2$.

As is well known, Hamiltonians with chiral symmetry can take an off-diagonal block form [56]. We have treated the chiral operator of the form $\sigma_1 \otimes 1$. However, we may choose to express the chiral operator as $\sigma_3 \otimes 1$, which is known as a canonical expression of the chiral operator. In fact, since

$$h^{-1}\sigma_1 h = \sigma_3, \quad h = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$  

(192)

the matrix $\sigma_1 \otimes 1$ is unitarily equivalent to $\sigma_3 \otimes 1$;

$$(h^{-1} \otimes 1)(\sigma_1 \otimes 1)(h \otimes 1) = \sigma_3 \otimes 1.$$  

(193)

It is easy to verify that the unitary matrix $g = h \otimes 1$ brings the $Q$ matrices (191) into an off-diagonal block form,

$$gQ_{\pm}g^{-1} = \frac{1}{\lambda^\pm} \begin{pmatrix} 0 & \mu \sigma \mp i k \cdot \sigma \\ \mu \sigma \pm i k \cdot \sigma & 0 \end{pmatrix}, \quad g = h \otimes 1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$  

(194)

respectively.

### 4.4 Mappings of $\mathbb{R}^3$ to $S^3$

From (194), we may pick up the off-diagonal block matrices

$$\frac{1}{\lambda^\pm} (\mu \sigma \pm i k \cdot \sigma).$$  

(195)

Since

$$\det\left(\frac{1}{\lambda^\pm} (\mu \sigma \pm i k \cdot \sigma)\right) = \frac{1}{|\lambda|^2} \det(\mu \sigma \pm i k \cdot \sigma) = 1,$$  

(196)

these matrices lie in $SU(2) \cong S^3$. Since the multiplication of (195) by $\pm i$ gives no topological change, we are allowed to take, independently of the choice of $Q_{\pm}$, the mappings

$$k \mapsto \frac{1}{|\lambda^\pm|} (k \cdot \sigma \pm i \mu), \quad \lambda^\pm = \frac{1}{|\lambda^\pm|} \begin{pmatrix} k_3 \pm i \mu \\ k_1 \pm i k_2 \\ k_2 \pm i k_1 \end{pmatrix},$$  

(197)

and to regard this mapping as defining the mapping of $\mathbb{R}^3$ to $S^3$,

$$q_{\pm}: k \mapsto \frac{1}{\sqrt{k^2 + \mu^2}} \begin{pmatrix} k_1 + ik_2 \\ k_3 \pm i \mu \\ k_2 \pm i k_1 \end{pmatrix} \in S^3 \subset \mathbb{C}^2 \cong \mathbb{R}^4,$$  

(198)

where the identification $\mathbb{C}^2 \cong \mathbb{R}^4$ is defined through

$$(x_1 + ix_2, x_3 + ix_4) \mapsto (x_1, x_2, x_3, x_4).$$  

(199)
4.5 Mapping degrees or winding numbers

We first study the mapping

\[ q_+ (k) = \frac{1}{\sqrt{k^2 + \mu^2}} \left( \frac{k_1 + ik_2}{k_3 + i\mu} \right) \in S^3 \subset \mathbb{C}^2 \cong \mathbb{R}^4. \]  

(200)

If we let \( k = |k| \to \infty \), the limit points of the mapping (200) are expressed as

\[ q_+ (k) = \frac{k}{\sqrt{k^2 + \mu^2}} \left( \frac{(k_1 + ik_2)/k}{(k_3 + i\mu)/k} \right) \to \left( \frac{n_1 + in_2}{n_3} \right) \in S^2 \subset S^3, \]  

(201)

where \( S^2 \) denotes the equator of the \( S^3 \), to which the vector \( n = (n_k) \) belongs.

Figure 7: A schematic description of \( q_+ (k) \)

Let \( \mathbb{R}^3_\mu \) denote the three-plane parallel to the tangent plane to the unit sphere \( S^3 \) at the north or south pole, intersecting the fourth axis at \((0, \mu) \in \mathbb{R}^3 \times \mathbb{R} \). The mapping \( q_+ (k) \) given in (200) maps each point \((k, \mu)\) on the plane \( \mathbb{R}^3_\mu \) to the point at which the line joining \((k, \mu)\) and the origin crosses the unit sphere \( S^3 \) (see Fig. 7). Equations (200) and (201) imply that if \( \mu > 0 \) the upper hemisphere is covered by \( \mathbb{R}^3_\mu \) through the mapping \( q_+ \) and if \( \mu < 0 \) the lower hemisphere is covered. It is to be noted that if \( \mu < 0 \) the orientation of the lower hemisphere covered by the mapping is opposite to the naturally defined orientation of \( S^3 \).

We proceed to discuss the mapping degree of (200) in terms of integrals over \( \mathbb{R}^3 \). We have to start by finding the area element of the sphere \( S^3 \subset \mathbb{R}^4 \). Let \((x_k)\) be the Cartesian coordinates of \( \mathbb{R}^4 \). The area element of \( S^3 \) is obtained by contracting the canonical volume element \( dx_1 \wedge dx_2 \wedge dx_3 \wedge dx_4 \) by the radial vector field \( \sum x_k \partial / \partial x_k \). In view of the orientation of the tangent plane to \( S^3 \) at the north pole, we take the area element of \( S^3 \) as

\[ \omega = -x_1 dx_2 \wedge dx_3 \wedge dx_4 + x_2 dx_3 \wedge dx_4 \wedge dx_1 - x_3 dx_4 \wedge dx_1 \wedge dx_2 + x_4 dx_1 \wedge dx_2 \wedge dx_3. \]  

(202)

The pull-back \( q_+^* \omega \) of the area form \( \omega \) is shown to take the form

\[ q_+^* \omega = \frac{\mu dk_1 \wedge dk_2 \wedge dk_3}{(k^2 + \mu^2)^2}. \]  

(203)
Introducing the spherical polar coordinates \((k, \theta, \phi)\) in the \(k\)-space \(\mathbb{R}^3\), we integrate \(q_+^* \omega\) over \(\mathbb{R}^3\) to obtain
\[
\int_{\mathbb{R}^3} q_+^* \omega = \pi^2 \frac{\mu}{|\mu|}.
\] (204)

Since \(\text{vol}(S^3) = 2\pi^2\), the mapping degree of \(q_+ : \mathbb{R}^3 \to S^3\) is defined and evaluated as
\[
\nu[q_+] = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} q_+^* \omega = \frac{1}{2} \frac{\mu}{|\mu|}.
\] (205)

The factor \(\frac{1}{2}\) implies that half of the sphere \(S^3\) is covered by the mapping \(q_+\), and \(\frac{\mu}{|\mu|} = \pm 1\) means that the covering is positively- or negatively-oriented according as \(\text{sgn}(\mu)\). This is completely in agreement with the schematic description of the mapping \(q_+\), which is already shown in Fig. 7.

We turn to the mapping
\[
q_-(k) = \frac{1}{\sqrt{k^2 + \mu^2}} \begin{pmatrix} k_1 + ik_2 \\ k_3 - i\mu \end{pmatrix}.
\] (206)

Since the expression of \(q_-(k)\) is obtained by replacing the parameter \(\mu\) in the definition of \(q_+(k)\) by \(-\mu\), the winding number of \(q_-\) is obtained by replacing \(\mu\) by \(-\mu\) in (205);
\[
\nu[q_-] = -\frac{1}{2} \frac{\mu}{|\mu|}.
\] (207)

Through the mapping \(q_-\), a point \((k, \mu)\) on the plane \(\mathbb{R}_\mu^3\) (see Fig. 8) is mapped to the point \((k, -\mu)\) once, and then mapped to the point at which the line joining the origin and the \((k, -\mu)\) crosses the unit sphere.

Figure 8: A schematic description of \(q_-(k)\)

In place of \(q_\pm\), we are allowed to consider the mappings
\[
h_\pm(k) = \frac{1}{\sqrt{k^2 + \mu^2}} (k \cdot \sigma \pm i\mu \mathbb{1}),
\] (208)

which also come from (197) and are viewed as mappings \(\mathbb{R}^3 \to SU(2)\). In what follows, we mainly treat \(h_+\).
The winding number (or mapping degree) of $h_+$ is defined to be

$$\nu[h_+] = \frac{1}{24\pi^2} \int_{SU(2)} \text{tr}(h_+^\dagger dh_+ \wedge h_+^\dagger dh_+ \wedge h_+^\dagger dh_+),$$

(209)

where $24\pi^2$ is the volume of $SU(2)$ with respect to the volume form determined by the left- or the right-invariant one-forms. This winding number for a mapping $\mathbb{R}^3 \rightarrow SU(2)$ is usually adopted in literature [56]. A straightforward but rather lengthy calculation with (208) provides

$$\text{tr}(h_+^\dagger dh_+ \wedge h_+^\dagger dh_+ \wedge h_+^\dagger dh_+) = \frac{12\mu}{(k^2 + \mu^2)^2} dk_1 \wedge dk_2 \wedge dk_3.$$  

(210)

Then, we obtain

$$\nu[h_+] = \frac{1}{24\pi^2} \int_{\mathbb{R}^3} \frac{12\mu dk_1 dk_2 dk_3}{(k^2 + \mu^2)^2} = \frac{1}{2} \frac{\mu}{|\mu|}$$

(211)

which is exactly the same as $\nu[q_+]$.

4.6 Jump in the mapping degree against the parameter

Though the mapping degrees $\nu[q_+]$ and $\nu[q_-]$ are half-integer valued, the change accompanying the variation in $\mu$ is integer valued;

$$\nu[q_+]|_{\mu>0} - \nu[q_-]|_{\mu<0} = \pm 1.$$  

(212)

We show that the jump (212) has a topological meaning. Since $q^*_+\omega$ is a three-form on $\mathbb{R}^3$, and since $\mathbb{R}^3$ is simply connected, $q^*_+\omega$ must be an exact form. We express $q^*_+\omega$, in terms of the polar spherical coordinates $(k, \theta, \phi)$, as

$$q^*_+\omega = \mu k \frac{2\sin \theta d\theta}{(k^2 + \mu^2)^2} \wedge \sin \theta d\theta \wedge d\phi.$$  

(213)

Denoting the canonical volume (or area) element on $S^2$ by

$$\varpi = \sin \theta d\theta \wedge d\phi,$$  

(214)

we can easily verify that $q^*_+\omega$ takes the form

$$q^*_+\omega = \mu d(F\varpi),$$  

(215)

where

$$F(k) = -\frac{k}{2(k^2 + \mu^2)} + \frac{1}{2\mu} \arctan \frac{k}{\mu}.$$  

(216)

Let $S_r$ denote the boundary of the ball $B_r$ of radius $r$ with the center at the origin. Then, the integral of $q^*_+\omega$ over $\mathbb{R}^3$ is evaluated as

$$\int_{\mathbb{R}^3} q^*_+\omega = \lim_{r \to \infty} \int_{B_r} q^*_+\omega = \lim_{r \to \infty} \mu F(r) \int_{S^2} \varpi,$$  

(217)
where $S^2$ denote the unit two-sphere, which may be viewed as the equator of $S^3$, the limit of $q_+(S_r)$ as $r \to \infty$. In the limit as $r \to \infty$, one obtains from (216)

$$\lim_{r \to \infty} \mu F(r) = \frac{\pi}{4} \text{sgn}(\mu),$$

so that the mapping degree of $q_+$ is put in the form

$$\nu[q_+] = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} q_+^* \omega = \frac{1}{8\pi} \text{sgn}(\mu) \int_{S^2} \varpi.$$  

(219)

When the parameter $\mu$ passes the zero value in the positive direction, the present equation provides the accompanying jump in the mapping degree as

$$\nu[q_+]|_{\mu>0} - \nu[q_+]|_{\mu<0} = \frac{1}{4\pi} \int_{S^2} \varpi.$$  

(220)

The right-hand side of the above equation is one, of course. We are allowed to interpret that the right-hand side is a topological quantity assigned to the equator $S^2$ as the limit of $q_+(S_r)$ as $r \to \infty$.

For the mapping $q_-(k)$ given in (206), we obtain, in place of (219),

$$\nu[q_-] = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} q_-^* \omega = -\frac{1}{8\pi} \text{sgn}(\mu) \int_{S^2} \varpi,$$

(221)

and in place of (220),

$$\nu[q_-]|_{\mu>0} - \nu[q_-]|_{\mu<0} = -\frac{1}{4\pi} \int_{S^2} \varpi.$$  

(222)

5 Correspondence between spectral flow and mapping degree

We are now in a position to answer the question, raised in Introduction, as to the correspondence between band rearrangement and topological change or the bulk-edge correspondence. In order to characterize the band rearrangement resulting from the 3D Dirac equation with the APS and the chiral bag boundary conditions, we have introduced the notion of spectral flow and its extension in Sec. 3.11 and found that the spectral flow in both cases of the APS and the chiral bag boundary conditions is $+1 + (-1) = 0$, where the spectral flow is taken as the ordinary or the extended one according as the APS or the chiral bag boundary condition is concerned. As we have already seen in Sec. 3.11, the zero value of the spectral flow does not mean a trivial phenomenon but implies that the redistribution of edge state eigenvalues takes place in opposite manners at the same time, independently of the choice of boundary conditions. We note in addition that the spectral flow is independent of the radius $R$ of the ball.

A semi-quantum counterpart to the spectral flow of the full quantum model has been discussed in Sec. 4.6 in terms of the mapping degree $\nu[q_\pm]$. As we have already found, the change in the mapping degree for each of $\nu[q_\pm]$ is given in (212) and interpreted as a winding number for the unit two-sphere (see (220) and (222)). The jumps
\[ \nu[q_+]_{\mu>0} - \nu[q_+]_{\mu<0} = 1 \quad \text{and} \quad \nu[q_-]_{\mu>0} - \nu[q_-]_{\mu<0} = -1 \]
can be viewed as corresponding to the eigenvalue transfer for the state with \( P < 0 \) and for the state with \( P > 0 \), respectively (see Fig. 6). The sum of the jumps is zero, of course.

It then turns out that the zero sum of the jumps in winding numbers (or mapping degrees) for the semi-quantum model is in marked correspondence to the zero spectral flow for the full quantum model. Since the semi-quantum Hamiltonian \( K_\mu \) is viewed as a bulk Hamiltonian (see Sec. 3.12), the correspondence between spectral flow and a change in mapping degree can be looked upon as a bulk-edge correspondence.

In order to get a better understanding of the correspondence between band rearrangement and topological change, we compare the respective correspondences for the 2D and the 3D models. The spectral flow for the 2D Dirac equation under both the APS and the chiral bag boundary conditions is \(+1\) or \(-1\) [39, 40] but the spectral flow for 3D Dirac equation is \(+1 - 1 = 0\). Correspondingly, the delta-Chern characterized as a winding number for \( S^1 \) in the 2D semi-quantum model takes value \(-1\) or \(+1\) according as the eigenvalue is positive or negative [40], but the changes in winding numbers for \( S^2 \) in the 3D semi-quantum model take values \( \pm 1 \) independently of the sign of the eigenvalue and the sum of those values is zero. Here, we notice that the \( S^1 \) and \( S^2 \) referred to in the 2D and the 3D semi-quantum models are viewed as the equator of \( S^2 \) and of \( S^3 \), respectively. Though the correspondence between band rearrangement and topological change hold true for the 2D and the 3D models, the difference in appearance comes from the difference in the discrete symmetries that the Hamiltonians in respective models admit.

### 6 Concluding remarks

In Sec. 2, we did not refer to the AZ classification [3, 26] of Hermitian matrices for brevity. We here make remarks on the nomenclature such as \( A, \text{AI}, \text{AII}, \text{AIII}, \text{etc.} \), used in the AZ classification. These symbols come from the classification of symmetric spaces by Cartan (see [27]). The classes \( A, \text{AI}, \text{AII} \) are called the Wigner-Dyson classes [61, 17], and classified with respect to the time-reversal operator: Matrices belonging to the class \( A \) are merely Hermitian. If a Hermitian matrix admits the time-reversal symmetry, it belongs to the class \( \text{AI} \) or \( \text{AII} \), according to whether the squared time-reversal operator is equal to the identity or to minus the identity. The Hamiltonian \( \mathcal{H} \) given in (6) belongs to the class \( \text{AII} \), since the squared time-reversal operator is equal to minus the identity; \((\mathbb{1} \otimes i\sigma_2)K)^2 = -\text{id}_{C_2 \otimes C_2}\). If we further require \( \mathcal{H} \) to admit the \( SU(2) \) symmetry, in the form different from (12), by imposing that

\[
(\mathbb{1} \otimes g)\mathcal{H}(\mathbb{1} \otimes g)^{-1} = \mathcal{H}, \quad g \in SU(2),
\]

the Hamiltonian becomes a real symmetric matrix,

\[
\mathcal{H} = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \otimes \mathbb{1}, \; a_{jk} \in \mathbb{R},
\]

which naturally reduces to a \( 2 \times 2 \) real symmetric matrix. Hamiltonians of this form belong to the class \( \text{AI} \), since the squared time-reversal operator is the identity, where the relevant time-reversal operator is merely the complex conjugation.
In addition, since the semi-quantum Hamiltonian $K_{\mu}(k)$ admits the chiral symmetry, it belongs to the class AIII, where Hamiltonians having the chiral symmetry are classified into AIII without reference to the time-reversal or the particle-hole symmetry. Further, on account of the particle-hole symmetry with $((\sigma_1 \otimes i\sigma_2)K)^2 = -\text{id}_{C^2 \otimes C^2}$, it belongs to the class CII, where Hamiltonians having the chiral symmetry are classified into CII without reference to the time-reversal or the particle-hole symmetry. Further, on account of the particle-hole symmetry with $((\sigma_1 \otimes i\sigma_2)K)^2 = -\text{id}_{C^2 \otimes C^2}$ and the time-reversal symmetry with $((\mathbb{1} \otimes i\sigma_2)K)^2 = -\text{id}_{C^2 \otimes C^2}$.

We have to compare the conditions (12) and (223) concerning $SU(2)$ symmetry. Since distinction among parameters of a Hamiltonian is not required in the AZ classification, Eq. (223) is adopted as a symmetry condition. However, parameters of a semi-quantum Hamiltonian in this article have to be broken up into control parameters and dynamical variables, so that (12) has been adopted as a symmetry condition, while we have called (12) $SU(2)$-equivariant.

We here recall that we have imposed the chiral symmetry in addition to the time-reversal symmetry in order to characterize the semi-quantum Hamiltonian $K_{\mu}(k)$ given in (4). In contrast to this, if we do not impose the chiral symmetry but merely require the Hermitian matrix (6) to be traceless, the Hamiltonian admitting the time-reversal symmetry proves to take the form

$$\tilde{K}_{\mu}(k, k_4) = \begin{pmatrix} \mu \mathbb{1} & k_4 \mathbb{1} - i\mathbf{k} \cdot \sigma \\ k_4 \mathbb{1} + i\mathbf{k} \cdot \sigma & -\mu \mathbb{1} \end{pmatrix}, \quad (k, k_4) \in \mathbb{R}^4,$$

(225)

where the parameters in (6) have been replaced according to $a = k_4 - ik_3, b = -k_2 - ik_1, c = \mu$ and $d = -\mu$. A comparison of (225) with (4) or (9) shows that the chiral symmetry makes the semi-quantum Hamiltonian $\tilde{K}_{\mu}(k, k_4)$ defined on $\mathbb{R}^4$ reduce to the $K_{\mu}(k)$ defined on $\mathbb{R}^3$. Furthermore, if $k_j, j = 1, \ldots, 4$, are replaced by $-i\partial/\partial x_j$, the $\tilde{K}_{\mu}$ brings about the 4D Dirac Hamiltonian defined on $\mathbb{R}^4$. A question as to the correspondence between band rearrangement and topological change for the 4D Dirac Hamiltonian is reserved for a future study.

An additional question is raised as for the correspondence between band rearrangement in a full quantum model and topological change in the corresponding semi-quantum model. The conclusion described in Sec. 5 was obtained through the free Dirac equation defined on the bounded domain, irrespective of the choice of the APS and the chiral bag boundary conditions. The additional question is as to whether a similar correspondence holds true or not if a full quantum model is defined on an unbounded domain, say $\mathbb{R}^2$ or $\mathbb{R}^3$, in the presence of an electric or magnetic field.

Last but not least, we remark that classification schemes for vector bundles have been studied according to the AZ classification [13, 14].
A  Spinor harmonics and the Hamiltonian in the polar spherical coordinates

We make a brief review of the representation spaces for the orbital angular momentums. As is well known, the spherical harmonics on \( S^2 \) are given by

\[
Y_{\ell}^m(\theta, \phi) = (-1)^m \sqrt{\frac{2\ell + 1}{4\pi}} \sqrt{\frac{(\ell - n)!}{(\ell + n)!}} \epsilon^{in\phi} P_{\ell}^n(\cos \theta),
\]

where \( P_{\ell}^n(x) \) are the associated Legendre functions defined to be

\[
P_{\ell}^n(x) = \frac{1}{2\ell!} (1 - x^2)^{n/2} \frac{d^{\ell+n}}{dx^{\ell+n}}(x^2 - 1)^\ell, \quad |n| \leq \ell.
\]

Further, the associated Legendre functions are known to satisfy the recursion formulas

\[
\begin{align*}
(\nu + \mu + 1)xP_\nu^\mu(x) - \sqrt{1 - x^2}P_{\nu + 1}^\mu(x) &= (\nu - \mu + 1)P_\nu^\mu(x), \\
xP_\nu^\mu(x) + (\nu + \mu)\sqrt{1 - x^2}P_{\nu - 1}^\mu(x) &= P_\nu^\mu(x), \\
xP_\nu^\mu(x) - (\nu - \mu + 1)\sqrt{1 - x^2}P_{\nu - 1}^\mu(x) &= P_{\nu + 1}^\mu(x), \\
(\nu - \mu)xP_\nu^\mu(x) + \sqrt{1 - x^2}P_{\nu + 1}^\mu(x) &= (\nu + \mu)P_{\nu - 1}^\mu(x).
\end{align*}
\]

We recall also that the orbital angular momentum operators \( L_k \) acts on \( Y_{\ell}^m \) according to

\[
\begin{align*}
(L_1 + iL_2)Y_{\ell}^m &= \sqrt{\ell + n}(\ell + n + 1)Y_{\ell}^{m+1}, \\
(L_1 - iL_2)Y_{\ell}^m &= \sqrt{(\ell + n)(\ell - n + 1)}Y_{\ell}^{m-1}, \\
L_3Y_{\ell}^m &= mY_{\ell}^m.
\end{align*}
\]

On account of the formula \( P_\ell^m(-x) = (-1)^{n+\ell}P_\ell^m(x) \) and \( e^{in(\phi + \pi)} = (-1)^n e^{im\phi} \), the spherical harmonics have the parity

\[
Y_{\ell}^m(-\mathbf{r}) = (-1)^\ell Y_{\ell}^m(\mathbf{r}), \quad |\mathbf{r}| = 1.
\]

We now compose the basis spinors which are simultaneous eigenstates of \( J_3 \) and \( \mathbf{J}^2 \). For \( j = \ell + \frac{1}{2} \), the basis state of \( J_3 \) takes the form \((c_1Y_{\ell}^{m-\frac{1}{2}}, c_2Y_{\ell}^{m+\frac{1}{2}})^T\). In fact, we obtain

\[
\begin{pmatrix}
L_3 + \frac{1}{2} & 0 \\
0 & L_3 - \frac{1}{2}
\end{pmatrix}
\begin{pmatrix}
c_1Y_{\ell}^{m-\frac{1}{2}} \\
c_2Y_{\ell}^{m+\frac{1}{2}}
\end{pmatrix} = m
\begin{pmatrix}
c_1Y_{\ell}^{m-\frac{1}{2}} \\
c_2Y_{\ell}^{m+\frac{1}{2}}
\end{pmatrix}, \quad |m| \leq j = \ell + \frac{1}{2},
\]

where \( m \) take values of half-integers. The constants \( c_1, c_2 \) are to be determined by the condition that \((c_1Y_{\ell}^{m-\frac{1}{2}}, c_2Y_{\ell}^{m+\frac{1}{2}})^T\) is also an eigenstate of \( \mathbf{J}^2 \) together with the normalization condition \( |c_1|^2 + |c_2|^2 = 1 \). As is easily seen, the square \( \mathbf{J}^2 \) is written out as

\[
\mathbf{J}^2 = \begin{pmatrix}
L_1 + L_2 + \frac{3}{2} & L_1 - iL_2 \\
L_1 + iL_2 & L_2 - L_3 + \frac{3}{2}
\end{pmatrix}.
\]
Operating $\Phi = (c_1 Y^{m-\frac{1}{2}}_\ell, c_2 Y^{m+\frac{1}{2}}_\ell)^T$ with $J^2$, we obtain the condition for $\Phi$ to be an eigenstate associated with the eigenvalue $j(j+1)$ of $J^2$, which results in

$$\frac{c_1}{\sqrt{\ell + m + \frac{1}{2}}} = \frac{c_2}{\sqrt{\ell - m + \frac{1}{2}}}.$$  \hspace{1cm} (233)

This equation and the normalization condition for $c_1, c_2$ are put together to give the basis (31). For $j = (\ell + 1) - \frac{1}{2}$, in a similar manner, we find that

$$\frac{c_1}{\sqrt{\ell - m + \frac{3}{2}}} = -\frac{c_2}{\sqrt{\ell + m + \frac{3}{2}}}.$$  \hspace{1cm} (234)

With the normalization condition for $c_1, c_2$, we obtain the basis (32).

In the rest of this appendix, we make a brief review of the Dirac Hamiltonian expressed in terms of the polar spherical coordinates. As is well known, the standard moving frame attached to the polar spherical coordinates is given by

$$e_r = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}, \quad e_\theta = \begin{pmatrix} \cos \theta \cos \phi \\ \cos \theta \sin \phi \\ -\sin \theta \end{pmatrix}, \quad e_\phi = \begin{pmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{pmatrix},$$  \hspace{1cm} (235)

where $e_\theta$ and $e_\phi$ are defined on the domain without the $z$-axis or with $\theta \neq 0, \pi$. The associated vector fields (or operators) are expressed, respectively, as

$$e_r \cdot \nabla = \frac{\partial}{\partial r}, \quad e_\theta \cdot \nabla = \frac{1}{r} \frac{\partial}{\partial \theta}, \quad e_\phi \cdot \nabla = \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi},$$  \hspace{1cm} (236)

where $\nabla$ denotes the ordinary gradient operator.

By using the identity

$$e_r e_r^T + e_\theta e_\theta^T + e_\phi e_\phi^T = \text{id}_{\mathbb{R}^3},$$  \hspace{1cm} (237)

where the superscript $^T$ denotes the transposition, we can put the Dirac Hamiltonian (3) in the form

$$H = -i \gamma \cdot (e_r e_r^T + e_\theta e_\theta^T + e_\phi e_\phi^T) \nabla + \mu \gamma_0$$

$$= -i \gamma_0 \partial_r - \frac{i}{r} (\gamma_\theta X_\theta + \gamma_\phi X_\phi) + \mu \gamma_0,$$  \hspace{1cm} (238)

where

$$\gamma_a = \gamma \cdot e_a, \quad a \in \{r, \theta, \phi\},$$  \hspace{1cm} (239a)

$$\frac{1}{r} X_b = e_b \cdot \nabla, \quad b \in \{\theta, \phi\},$$  \hspace{1cm} (239b)

and where the operators $X_b$ are determined through (236) and (239b). We here remark that the products among $\sigma_a$ and among $\gamma_a$, $a \in \{r, \theta, \phi\}$ are given by

$$\sigma_a \sigma_b = i \sigma_b, \quad \sigma_\theta \sigma_\phi = i \sigma_\phi, \quad \sigma_\phi \sigma_\theta = i \sigma_\theta, \quad \sigma_r^2 = \sigma_\theta^2 = \sigma_\phi^2 = 1,$$  \hspace{1cm} (240)
\[ \gamma_r \gamma_\theta = i \mathbb{1} \otimes \sigma_r, \quad \gamma_\theta \gamma_\phi = i \mathbb{1} \otimes \sigma_\theta, \quad \gamma_\phi \gamma_r = i \mathbb{1} \otimes \sigma_\phi, \quad \gamma_r^2 = \gamma_\theta^2 = \gamma_\phi^2 = \mathbb{1} \otimes \mathbb{1}, \tag{241} \]

respectively, and they satisfy
\[ \sigma_a \sigma_b + \sigma_b \sigma_a = 2 \delta_{ab} \mathbb{1}, \quad a, b \in \{r, \theta, \phi\}, \tag{242} \]
\[ \gamma_a \gamma_b + \gamma_b \gamma_a = 2 \delta_{ab} \mathbb{1} \otimes \mathbb{1}, \quad a, b \in \{r, \theta, \phi\}, \tag{243a} \]
\[ \gamma_a \gamma_0 + \gamma_0 \gamma_a = 0. \tag{243b} \]

Further calculation with the above formula provides
\[
\begin{align*}
- \frac{i}{r} \gamma_r (\gamma_\theta X_\theta + \gamma_\phi X_\phi) + \mu \gamma_r \gamma_0 &= \frac{i}{r} \begin{pmatrix}
- i \sigma_\theta X_\theta + i \sigma_\theta X_\phi & \mu r \sigma_r \\
\mu r \sigma_r & - i \sigma_\phi X_\theta + i \sigma_\theta X_\phi
\end{pmatrix} \\
&= \frac{i}{r} \begin{pmatrix}
\sigma \cdot L & \sigma \cdot r \\
\sigma \cdot r & \sigma \cdot L
\end{pmatrix}, \tag{244}
\end{align*}
\]

where use has been made of
\[
\begin{align*}
L_1 + i L_2 &= e^{i \phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right), \tag{245a} \\
L_1 - i L_2 &= - e^{-i \phi} \left( \frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right), \tag{245b} \\
L_3 &= - i \frac{\partial}{\partial \phi}. \tag{245c}
\end{align*}
\]

and
\[
\begin{align*}
i (\sigma_\phi X_\theta - \sigma_\theta X_\phi) &= - \begin{pmatrix}
L_3 \\
L_1 + i L_2 \\
- i L_2 \\
- L_3
\end{pmatrix} = - \sigma \cdot L. \tag{246}
\end{align*}
\]

Eqs. (238) and (244) together with \( \gamma_r^2 = \mathbb{I} \) are combined to provide (43).

**Acknowledgements.** The authors would like to thank Dr. G. Dhont for drawing graphs of bulk and edge state eigenvalues as functions of the control parameter and as those of the angular momentum eigenvalue as well. Part of this work was supported by a Grant-in-Aid for Scientific Research 18K03297 (T.I) from JSPS.

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