Position space formulation for Dirac fermions on honeycomb lattice

Masaki Hirotsu\textsuperscript{1} \textsuperscript{a}, Tetsuya Onogi\textsuperscript{1} \textsuperscript{b} and Eigo Shintani\textsuperscript{2} \textsuperscript{c}

\textsuperscript{1}Department of Physics, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
\textsuperscript{2}RIKEN-BNL Research Center, Brookhaven National Laboratory, Upton, NY 11973, USA

Abstract

We study how to construct Dirac fermion defined on the honeycomb lattice in position space. Starting from the nearest neighbor interaction in tight binding model, we show that the Hamiltonian is constructed by kinetic term and second derivative term of three flavor Dirac fermions in which one flavor has a mass of cutoff order and the other flavors are massless. In this formulation the structure of the Dirac point is simplified so that its uniqueness can be easily shown even if we consider the next-nearest neighbor interaction. We also explicitly show that there exists an exact chiral symmetry at finite lattice spacing, which protects the masslessness of the Dirac fermion, and discuss the analogy with the staggered fermion formulation.
1 Introduction

Graphene forms from a layer of carbon atoms with hexagonal tiling \(^1\) and it is much discussed in not only condensed matter physics but also high energy physics for its remarkable features \(^2\). One of the most important features of graphene is that the quasiparticles behave like massless Dirac fermion with effective speed of light near \(c/300\) \(^3\). An explanation to the question why massless Dirac fermion emerges in non-relativistic many body system was primarily given by Semenoff \(^4\). Ref. \(^4\) has shown that the low energy excitations around two independent Dirac points on the fermi-surface can be described by two relativistic Weyl fermions having opposite chiralities, which are also regarded as massless Dirac fermion. However, since this construction is based on the momentum space representation, it is not clear how one can introduce the effect of gauge interaction as local interactions.

In this paper we show the construction of Dirac fermion from honeycomb lattice in position space, which allows one to introduce local gauge interactions and perform the dynamical calculation of physical observables. Furthermore in this formulation the structure of flavor symmetry becomes manifest, and we can easily identify the quantum number of low energy excitations. We also expect that the formulation enables to advance a study of the dynamical nature of graphene such as the gap generation, which is associated with the spontaneous breakdown of chiral symmetry.

This paper is organized as follows. In section \(2\) we briefly review the construction of Dirac fermion from honeycomb lattice in momentum space. In section \(3\) after introducing the formulation defined in position space, we discuss uniqueness of Dirac point and physical modes, and then we show that two massless Dirac fermion appear at low energy region in section \(4\). In section \(5\), we discuss a derivation of exact chiral symmetry in our formulation, and the last section is devoted to the summary and discussion.

2 The conventional derivation from honeycomb lattice

We first review the conventional derivation of Dirac fermion formulation from tight binding model of honeycomb lattice \(^4, 8\). Let us start from the tight binding Hamiltonian

\[
H = \sum_{\vec{r},i=1,2,3} \sum_{\sigma} \left[ a^\dagger_\sigma(\vec{r}) b_\sigma(\vec{r} + \vec{s}_i) + b^\dagger_\sigma(\vec{r}) a_\sigma(\vec{r}) \right] - t' \sum_{\vec{r},i=1,2,3} \sum_{\sigma} \left[ a^\dagger_\sigma(\vec{r} + \vec{s}_i) b_\sigma(\vec{r}) \right],
\]

where the first line is a nearest neighbor hopping term and the second line is a next nearest neighbor hopping term, and \(t, t'\) are hopping amplitudes. \(a^\dagger, a\) and \(b^\dagger, b\) are the fermionic creation and annihilation operators of electrons on two triangular sublattices A and B in
Figure 1: Honeycomb lattice is constituted of two triangular sub-lattices A and B, which are colored with red and blue respectively.

Figure 1. $\vec{s}_i (i = 1, 2, 3)$ and $\vec{s}_j '(j = 1, \cdots , 6)$ denote the relative position vectors for three nearest neighbors, and for the six next-to-nearest neighbors respectively, and $\vec{s}_i (i = 1, 2, 3)$ are given explicitly by

$$\vec{s}_1 = a_0 \left( 1, \ 0 \right), \ \vec{s}_2 = a_0 \left( -1/2, \ \sqrt{3}/2 \right), \ \vec{s}_3 = a_0 \left( -1/2, \ -\sqrt{3}/2 \right),$$

where $a_0$ is a lattice spacing. We note that in graphene system above parameters are given as $t = 2.8$ eV and $t' = 0.1$ eV [9], and $a_0 = 1.42$ Å [2]. In the following discussion we take $t' = 0$ and also suppress spin index $\sigma$. In order to consider Dirac point on fermi-surface, the Fourier transformation

$$a(\vec{r}) = \int \frac{d^2 k}{(2\pi)^2} e^{i\vec{k} \cdot \vec{r}} a(\vec{k}), \ b(\vec{r}) = \int \frac{d^2 k}{(2\pi)^2} e^{i\vec{k} \cdot \vec{r}} b(\vec{k})$$

for the fermionic creation and annihilation operator is usually employed, and thus the Hamiltonian in momentum space is given by

$$\mathcal{H} = \int \frac{d^2 k}{(2\pi)^2} \begin{pmatrix} \hat{a}(\vec{k}) & 0 \\ 0 & D^*(\vec{k}) \end{pmatrix} \begin{pmatrix} 0 & D(\vec{k}) \\ D^*(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} \hat{a}(\vec{k}) \\ \hat{b}(\vec{k}) \end{pmatrix}$$

with

$$D(\vec{k}) = t \sum_{i=1,2,3} e^{i\vec{k} \cdot \vec{s}_i}.$$  

The energy eigenvalue of the above Hamiltonian is represented as

$$E(\vec{k}) = \pm t \left| \sum_{i=1,2,3} e^{i\vec{k} \cdot \vec{s}_i} \right|.$$
In the half filling electron system, the negative and positive eigenvalues corresponding to the valence band and conduction band respectively appear, and it turns out that there exist two independent Dirac points $\vec{K}_\pm$ on the fermi-surface, which satisfy $E(\vec{K}_\pm) = 0$.

In order to derive the low energy effective Hamiltonian, we expand $D(\vec{k})$ around the Dirac points to first order of momentum $\vec{p}$. Regarding $\vec{K}_\pm$ and A, B site as spin degrees of freedom (DOF), and defining 4-components spinor $\tilde{\xi}(\vec{p})$ as

$$\tilde{\xi}(\vec{p}) = (\tilde{a}(\vec{K}_+ + \vec{p}), \tilde{b}(\vec{K}_+ + \vec{p}), \tilde{b}(\vec{K}_- + \vec{p}), \tilde{a}(\vec{K}_- + \vec{p}))^T,$$

the Hamiltonian in Eq.(4) reads

$$H \approx iv \sum_{i=1,2} \int \frac{d^2p}{(2\pi)^2} \tilde{\xi}^\dagger(\vec{p}) [\gamma_0 \gamma_i p_i] \tilde{\xi}(\vec{p}).$$

Here $v = 3a_0 t/2$ is interpreted as a fermi velocity of quasiparticles, and the matrices $\gamma_0, \gamma_1, \gamma_2$ satisfy Clifford algebra \{\$\gamma_\mu, \gamma_\nu\} = g_{\mu\nu} \cdot 1_{4 \times 4}$, where $g_{\mu\nu}$ is a metric in $2 + 1$ dimensional space-time. Further, introducing additional matrix $\gamma_3$, which anti-commutes with the above $\gamma_0, \gamma_1, \gamma_2$, we can define $\gamma_5 = i \gamma_0 \gamma_1 \gamma_2 \gamma_3$, which is a generator of chiral symmetry forbidding a (parity-invariant) mass term $m \tilde{\xi}^\dagger \gamma_0 \tilde{\xi}$.

In the next section we will show an alternative derivation of Dirac fermion based on position space, which has manifest locality and chiral symmetry.

3 Formulation in position space on honeycomb lattice

3.1 Tight binding model on the real space lattice

In this section, we explain our formulation and address Dirac point and physical modes. First we consider the labeling of DOF of the fermionic creation and annihilation operator as shown in Figure 2. In this labeling we define $A_\rho$ and $B_\rho$ ($\rho = 0, 1, 2$) as the new DOF having the operators on the site of honeycomb lattice and the argument of operator location is defined as the position of center of hexagonal unit cell with position vector $\vec{e}_\rho$ ($\rho = 0, 1, 2$). Thus in our formulation the tight binding Hamiltonian is expressed as

$$\mathcal{H} = \sum_{\vec{x}, \vec{y}} \sum_{\rho, \rho'} \left( \begin{array}{c} \chi_{A\rho}(\vec{x}) \\ \chi_{B\rho}(\vec{x}) \end{array} \right)^\dagger \left( \begin{array}{cc} t' \Pi(\vec{x}, \vec{y})_{\rho\rho'} & t \Phi(\vec{x}, \vec{y})_{\rho\rho'} \\ t \Phi(\vec{x}, \vec{y})_{\rho\rho'}^\dagger & t' \Pi(\vec{y}, \vec{x})_{\rho\rho'} \end{array} \right) \left( \begin{array}{c} \chi_{A\rho'}(\vec{y}) \\ \chi_{B\rho'}(\vec{y}) \end{array} \right),$$

(9)
where $\Phi(\vec{x},\vec{y})$ and $\Pi(\vec{x},\vec{y})$ are given by

$$
\Phi(\vec{x},\vec{y}) = 
\begin{pmatrix}
T_0 & 1 & 1 \\
1 & T_1 & 1 \\
1 & 1 & T_2
\end{pmatrix}
_{\vec{x},\vec{y}},
$$

(10)

$$
\Pi(\vec{x},\vec{y}) = 
\begin{pmatrix}
0 & 1 + T_0 + T_1^\dagger & 1 + T_0 + T_2^\dagger \\
1 + T_0^\dagger + T_1 & 0 & 1 + T_1 + T_2^\dagger \\
1 + T_0^\dagger + T_2 & 1 + T_1^\dagger + T_2 & 0
\end{pmatrix}
_{\vec{x},\vec{y}},
$$

(11)

with

$$
(T_\rho)_{\vec{x},\vec{y}} = \delta_{\vec{x},\vec{y}} + \vec{e}_\rho, \quad (1)_{\vec{x},\vec{y}} = \delta_{\vec{x},\vec{y}}.
$$

(12)

Figure 2: Honeycomb lattice

Here $\vec{x}, \vec{y}$ denote lattice sites on the fundamental lattice, which is composed of hexagonal unit cells bounded by red circles in Figure 2, and basic vectors $\vec{e}_\rho(\rho = 0, 1, 2)$ are given by

$$
\vec{e}_0 = a \begin{pmatrix} 1, & 0 \end{pmatrix}, \quad \vec{e}_1 = a \begin{pmatrix} -1/2, & \sqrt{3}/2 \end{pmatrix}, \quad \vec{e}_2 = a \begin{pmatrix} -1/2, & -\sqrt{3}/2 \end{pmatrix},
$$

(13)

where $a$ is a lattice spacing as a distance between hexagonal unit cells and these vectors satisfy $\vec{e}_0 + \vec{e}_1 + \vec{e}_2 = 0$. \footnote{Here we note that there is following relation between $\vec{e}_\rho(\rho = 0, 1, 2)$ and $\vec{s}_i (i = 1, 2, 3)$:

$$
\vec{e}_0 = 3\vec{s}_1, \quad \vec{e}_1 = 3\vec{s}_2, \quad \vec{e}_2 = 3\vec{s}_3.
$$

(14)}
operators on the triangular sublattice $I(= A, B)$ of honeycomb lattice. And we note
\[
\Pi(\vec{x}, \vec{y}) = \sum_{\vec{z}} \Phi(\vec{x}, \vec{z}) \Phi^\dagger(\vec{z}, \vec{y}) - 3 \cdot 1_{3 \times 3}
\] (15)
holds, which will be useful later.

### 3.2 The nearest neighbor interaction

In this section we assume $t' = 0$ as the leading tight binding approximation, and we discuss the general representation of Eq.(9).

Let us introduce the first and second derivatives on the lattice,
\[
\nabla_\rho \chi(\vec{x}) = \frac{1}{2} (\chi(\vec{x} + \vec{e}_\rho) - \chi(\vec{x} - \vec{e}_\rho)),
\]
(16)
\[
\Delta_\rho \chi(\vec{x}) = \chi(\vec{x} + \vec{e}_\rho) + \chi(\vec{x} - \vec{e}_\rho) - 2\chi(\vec{x}).
\]
(17)
The leading order of Hamiltonian (9) is written as the following tensor product form;
\[
\mathcal{H} = t \sum_{\vec{x}} \chi^\dagger(\vec{x}) \left[ (\tau_1 \otimes M) \chi(\vec{x}) - i \sum_{\rho} (\tau_2 \otimes \Gamma_\rho)(\nabla_\rho \chi(\vec{x})) + \frac{1}{2} \sum_{\rho} (\tau_1 \otimes \Gamma_\rho)(\Delta_\rho \chi(\vec{x})) \right]
\] (18)
with
\[
\chi(\vec{x}) = (\chi_{A0}(\vec{x}), \chi_{A1}(\vec{x}), \chi_{A2}(\vec{x}), \chi_{B0}(\vec{x}), \chi_{B1}(\vec{x}), \chi_{B2}(\vec{x}))^T,
\]
(19)
and
\[
M = \begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\
\end{pmatrix},
\Gamma_0 = \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\end{pmatrix},
\Gamma_1 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0 \\
\end{pmatrix},
\Gamma_2 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 0 & 0 \\
\end{pmatrix}.
\]
(20)
It is clear that the first derivative term of Eq.(18) corresponds to kinetic term, and the second derivative term corresponds to flavor dependent Wilson-like term.

Next we discuss a constant mode which is the eigenmode of the first term of Eq.(18),
\[
\mathcal{M} = t \sum_{\vec{x}} \chi^\dagger(\vec{x}) (\tau_1 \otimes M) \chi(\vec{x})
= \sum_{\vec{x}} \sum_{\rho, \rho'} \begin{pmatrix}
\chi_{A\rho}(\vec{x}) \\
\chi_{B\rho}(\vec{x})
\end{pmatrix}^\dagger \begin{pmatrix}
0 & tM_{\rho\rho'} \\
0 & 0
\end{pmatrix} \begin{pmatrix}
\chi_{A\rho'}(\vec{x}) \\
\chi_{B\rho'}(\vec{x})
\end{pmatrix}.
\]
(21)
Using the diagonalization of mass matrix $tM$, the above equation is described as
\[
\mathcal{M} = \sum_{\vec{x}} \sum_{\rho, \rho'} \begin{pmatrix}
\psi_{A\rho}(\vec{x}) \\
\psi_{B\rho}(\vec{x})
\end{pmatrix}^\dagger \begin{pmatrix}
0 & (M^{\text{diag}})_{\rho\rho'} \\
0 & (M^{\text{diag}})_{\rho\rho'}
\end{pmatrix} \begin{pmatrix}
\psi_{A\rho'}(\vec{x}) \\
\psi_{B\rho'}(\vec{x})
\end{pmatrix},
\]
(22)
\[
M^{\text{diag}} = \begin{pmatrix}
3t & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]
(23)
with unitary transformation,
\[ \chi_{I\rho}(\vec{x}) = \frac{1}{\sqrt{3}} \sum_{\rho' = 0, 1, 2} e^{i2\pi \rho \rho' / 3} \psi_{I\rho'}(\vec{x}), \] (24)
and thus we interpret from the above diagonalization that the constant mode can be decomposed into two zero modes and one massive mode.

In order to prove the uniqueness of the Dirac point, we consider an eigenvalue equation of this Hamiltonian in momentum space. Using following Fourier representation of \( \chi_{I\rho}(\vec{x}) \),
\[ \chi_{I\rho}(\vec{x}) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec{k} \cdot \vec{x}} \tilde{\chi}_{I\rho}(\vec{k}), \] (25)
Hamiltonian (18) in momentum space is given by
\[ \mathcal{H} = \int \frac{d^2k}{(2\pi)^2} \sum_{\rho, \rho'} \left( \begin{array}{c} \tilde{\chi}_{A\rho}(\vec{k}) \\ \tilde{\chi}_{B\rho}(\vec{k}) \end{array} \right) \mathcal{M} \left( \begin{array}{c} \tilde{\Phi}(\vec{k})_{\rho \rho'} \\ \tilde{\Phi}^\dagger(\vec{k})_{\rho \rho'} \end{array} \right) \left( \begin{array}{c} \tilde{\chi}_{A\rho'}(\vec{k}) \\ \tilde{\chi}_{B\rho'}(\vec{k}) \end{array} \right), \] (26)
where
\[ \tilde{\Phi}(\vec{k}) = \left( \begin{array}{ccc} b_0 & 1 & 1 \\ 1 & b_1 & 1 \\ 1 & 1 & b_2 \end{array} \right) \] (27)
with \( b_\rho = \exp[-i\vec{k} \cdot \vec{e}_\rho] (\rho = 0, 1, 2) \). The eigenvalue equation can read into
\[ \left| -\lambda^2 \cdot 1_{3 \times 3} + \tilde{\Phi}(\vec{k}) \tilde{\Phi}^\dagger(\vec{k}) \right| = 0, \] (28)
where
\[ \tilde{\Phi}(\vec{k}) \tilde{\Phi}^\dagger(\vec{k}) = \left( \begin{array}{ccc} 3 & b_0 + b_1^* + 1 & b_0 + b_2^* + 1 \\ b_0^* + b_1 + 1 & 3 & b_1 + b_2^* + 1 \\ b_0^* + b_2 + 1 & b_1^* + b_2 + 1 & 3 \end{array} \right). \] (29)
Assuming the electron system is half-filling in which the Dirac point on fermi-surface should appear at \( \lambda = 0 \), we can derive the condition, which Dirac point fulfills, by the substitution of \( \lambda = 0 \) into the above eigenvalue equation; we solve an equation \( |\tilde{\Phi}(\vec{k}) \tilde{\Phi}^\dagger(\vec{k})| = 0 \) \footnote{In general the eigenvalue equation of Eq.(28) can be represented as
\[ F(\lambda^2) = 0, \quad F(x) = x^3 - 9x^2 - 3(z_k + z_k^*) x - |z_k - 3|^2, \] (30)
where \( z_k \) will be defined in Eq.(32).} Using \( b_0 b_1 b_2 = 1 \) (since \( \vec{e}_0 + \vec{e}_1 + \vec{e}_2 = 0 \)), we find a simple condition
\[ z_k = 3, \] (31)
where
\[ z_k = b_0 + b_1 + b_2 = e^{-i\vec{k} \cdot \vec{e}_0} + e^{-i\vec{k} \cdot \vec{e}_1} + e^{-i\vec{k} \cdot \vec{e}_2}, \] (32)
and from this condition we have
\[ e^{-i\vec{k} \cdot \vec{e}_0} = e^{-i\vec{k} \cdot \vec{e}_1} = e^{-i\vec{k} \cdot \vec{e}_2} = 1, \] (33)
which means \( \vec{k} = n_1 \vec{u}_1 + n_2 \vec{u}_2 \) \( n_1, n_2 \) : integer, therefore we prove that Dirac point appears only at \( \vec{k} = 0 \) within the BZ. It turns out that the constant mode provides unique Dirac point at \( \vec{k} = 0 \) in this formulation within the nearest neighbor hopping approximation in contrast to the traditional formulation in which there are two Dirac points at the edge of BZ (see the section 2).

### 3.3 The next-to-nearest neighbor interaction

Here we will confirm that the Dirac point explained in the previous subsection does not disappear if we add the next-to-nearest neighbor hopping term. Turning on \( t' \neq 0 \), the tight binding Hamiltonian (9) is written as
\[
\mathcal{H} = \sum_{\vec{x}, \vec{y}} \sum_{\rho, \rho'} \begin{pmatrix} \chi_{A\rho}(\vec{x}) \\ \chi_{B\rho}(\vec{x}) \end{pmatrix}^\dagger \begin{pmatrix} t' \sum_{\vec{z}} \Phi(\vec{x}, \vec{z}) \Phi^\dagger(\vec{y}, \vec{z}) & t \Phi(\vec{x}, \vec{y})_{\rho\rho'} \\ t \Phi(\vec{x}, \vec{y})_{\rho\rho'} & t' \sum_{\vec{z}} \Phi(\vec{x}, \vec{z}) \Phi^\dagger(\vec{x}, \vec{y}) \end{pmatrix} \begin{pmatrix} \chi_{A\rho'}(\vec{y}) \\ \chi_{B\rho'}(\vec{y}) \end{pmatrix} - 3t' \sum_{\vec{x}, \vec{y}, \rho, \rho'} \begin{pmatrix} \chi_{A\rho}(\vec{x}) \\ \chi_{B\rho}(\vec{x}) \end{pmatrix}^\dagger \begin{pmatrix} 1_{3 \times 3} & 0 \\ 0 & 1_{3 \times 3} \end{pmatrix} \begin{pmatrix} \chi_{A\rho'}(\vec{y}) \\ \chi_{B\rho'}(\vec{y}) \end{pmatrix},
\] (34)
where we substituted Eq.(15). The second line merely shifts the origin of energy, and does not affect the dynamics at all. Therefore we neglect the constant term in the following discussion.

When we naively consider constant mode as in the previous subsection, the mass matrix of this Hamiltonian becomes
\[
\begin{pmatrix}
3t' & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix}
\begin{pmatrix}
t & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix},
\] (35)

\(^{\text{Note that } \{\vec{u}_i\}_{i=1,2} \text{ is the basis vector of reciprocal lattice space, which is defined as } \vec{e}_i \cdot \vec{u}_j = 2\pi \delta_{ij} \text{ (} i, j = 1, 2 \).}\)
then transforming the same basis as $\psi_I(x)$ in Eq. (25), this matrix is given as

\[
\begin{pmatrix}
9t' & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
3t & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
3t & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
9t' & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

(36)

and thus two zero modes and one massive mode also appear. One may think this implies that Dirac point does not change even if the next-to-nearest neighbor hopping term is included. However, it is not so trivial whether the fermi-surface remains in vanishing energy level holding on the half-filling configuration.

In order to investigate in detail, we discuss the energy spectrum of the modified Hamiltonian in momentum space, which is expressed as

\[
\mathcal{H} = \int \frac{d^2k}{(2\pi)^2} \bar{\chi}^\dagger(\vec{k})[K(\vec{k})]\chi(\vec{k})
\]

(37)

with

\[
K(\vec{k}) = \begin{pmatrix}
t'\Phi(\vec{k})\Phi^\dagger(\vec{k}) & t\Phi(\vec{k}) \\
t\Phi^\dagger(\vec{k}) & t'\Phi^\dagger(\vec{k})\Phi(\vec{k})
\end{pmatrix}
\]

(38)

We diagonalize $\Phi(\vec{k})$ by the following bi-unitary transformation

\[
U_A\Phi(\vec{k})U_B^\dagger = \text{diag}(\phi_0, \phi_1, \phi_2),
\]

(39)

where $U_A, U_B$ are some unitary matrices and $\phi_i$ ($i = 0, 1, 2$) are real eigenvalues of $\Phi(\vec{k})$.

Performing unitary transformation $U = U_A \oplus U_B$, $K(\vec{k})$ is transformed into

\[
\hat{K}(\vec{k}) = \begin{pmatrix}
t'\phi_0^2 & 0 & 0 & t\phi_0 & 0 & 0 \\
0 & t'\phi_1^2 & 0 & 0 & t\phi_1 & 0 \\
0 & 0 & t'\phi_2^2 & 0 & 0 & t\phi_2 \\
t\phi_0 & 0 & 0 & t'\phi_0^2 & 0 & 0 \\
0 & t\phi_1 & 0 & 0 & t'\phi_1^2 & 0 \\
0 & 0 & t\phi_2 & 0 & 0 & t'\phi_2^2
\end{pmatrix},
\]

(40)

where $\phi_i^2$ ($i = 0, 1, 2$) are the eigenvalues of $\Phi(\vec{k})\Phi^\dagger(\vec{k})$, and satisfy the eigenvalue equation

\[
F(\phi_i^2) = 0,
\]

(41)

where $F(x)$ is defined in Eq. (30). Here, the eigenvalue equation of $\hat{K}(\vec{k})$ is expanded into

\[
\prod_{i=0,1,2} \left[ (\lambda' - t'\phi_i^2)^2 - t^2\phi_i^2 \right] = 0,
\]

(42)
where \( \lambda' \) is an eigenvalue of \( \hat{K}(\vec{k}) \), and we obtain

\[
E'_\pm(\phi_i) = t' \phi_i^2 \pm t|\phi_i|
\]

\[
= t' \phi_i^2 f_\pm(|\phi_i/\phi_c|)
\]

(43)

with \( \phi_c = t/t' \) and \( f_\pm(x) = x^2 \pm x \). In Eq. (43), taking \( t' = 0 \), the fermi-surface appears at vanishing energy level in the half-filled electron system since the number of positive eigenvalues \( E_+(\phi_i) = t|\phi_i| \) and the number of negative eigenvalues \( E_-(\phi_i) = -t|\phi_i| \) are the same.

However, taking account into the effect of the next-to-nearest neighbor hopping term, \( t' \neq 0 \), the situation turns less simple.

We plot \( E'_\pm(\phi_i)/t'\phi_c^2 \) against \( |\phi_i/\phi_c| \) in Figure 3. It is obvious that the number of eigenvalues \( E'_+(\phi_i) \) and that of \( E'_-(\phi_i) \) are also the same. In Figure 3, we see that the negative eigenvalues \( E'_-(\phi_i) \) remain in negative values unless \( |\phi_i| \) exceeds \( |\phi_c| \), while the eigenvalues \( E'_+(\phi_i) \) stay in positive values at arbitrary \( |\phi_i| \). Thus if \( |\phi_i| \) does not exceed the threshold, the fermi surface remains in vanishing energy since the number of the positive eigenvalues equals that of the negative eigenvalues. On the other hand, if \( |\phi_i| \) exceeds the threshold, the fermi surface stays no longer in the same energy level.

From the eigenvalue equation of \( \tilde{\Phi}(\vec{k})\tilde{\Phi}^\dagger(\vec{k}) \) in Eq. (41), the range of \( |\phi_i| \) is shown to be between 0 and 3. Therefore, when \( 3 < |\phi_c| \), the Dirac point is stable in adding the next-to-nearest neighbor hopping term. Especially in graphene system, the fermi surface is not changed since \( |\phi_c| \approx 28 \).

4 Close to the continuum limit

In this section, we show the derivation of Dirac fermion formulation in position space close to the continuum limit. Here we consider the low-energy expansion of Hamiltonian around Dirac point and investigate ”chiral” symmetry which forbids mass gap in low energy region.

In momentum space, the tight binding Hamiltonian in terms of the mass eigenstate is given as

\[
\mathcal{H} = \int \frac{d^2k}{(2\pi)^2} \sum_{a,a'} \left( \begin{array}{c} \tilde{\psi}_{Aa}(\vec{k}) \\ \tilde{\psi}_{Ba}(\vec{k}) \end{array} \right)^\dagger \left( \begin{array}{cc} 0 & \tilde{\Phi}'(\vec{k})_{aa'} \\ \tilde{\Phi}'(\vec{k})_{aa'}^\dagger & 0 \end{array} \right) \left( \begin{array}{c} \tilde{\psi}_{Aa'}(\vec{k}) \\ \tilde{\psi}_{Ba'}(\vec{k}) \end{array} \right),
\]

(44)

where \( \tilde{\psi}_{Ia}(\vec{k}) \) is a Fourier representation of the mass eigenstate of \( \psi_{Ia}(\vec{x}) \) and \( \tilde{\Phi}'(\vec{k}) \) denotes \( \tilde{\Phi}(\vec{k}) \) in basis of these mass eigenstates, which are defined as

\[
\tilde{\psi}_{Ia}(\vec{k}) = \sum_{\vec{x}} e^{-i\vec{k} \cdot \vec{x}} \psi_{Ia}(\vec{x}),
\]

(45)
Figure 3: x axis denotes $|\phi_i / \phi_c|$, and y axis denotes energy eigenvalues divided by $t' \phi_c^2$. The dashed lines colored with red and blue are $E_+(\phi_i)/t' \phi_c^2 = |\phi_i / \phi_c|$ and $E_- (\phi_i)/t' \phi_c^2 = -|\phi_i / \phi_c|$ respectively. While the solid lines colored with red and blue are $E'_+(\phi_i)/t' \phi_c^2 = f_+(|\phi_i / \phi_c|)$ and $E'_-(\phi_i)/t' \phi_c^2 = f_-(|\phi_i / \phi_c|)$.

\[
\tilde{\Phi}'(\vec{k}) = \frac{1}{3} \begin{pmatrix}
3 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} - \frac{a}{2} ik_1 \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix} - \frac{a}{2} ik_2 \begin{pmatrix}
0 & -i & i \\
i & 0 & -i \\
-i & i & 0
\end{pmatrix}
- \frac{a^2}{4} \begin{pmatrix}
k_1^2 + k_2^2 & (k_1 + ik_2)^2/2 & (k_1 - ik_2)^2/2 \\
(k_1 - ik_2)^2/2 & k_1^2 + k_2^2 & (k_1 + ik_2)^2/2 \\
(k_1 + ik_2)^2/2 & (k_1 - ik_2)^2/2 & k_1^2 + k_2^2
\end{pmatrix} + O(k^3),
\] (46)

Expanding $\tilde{\Phi}(\vec{k})$ with respect to momentum around Dirac point to the second order in $\vec{k}$ as

\[
\tilde{\Phi}(\vec{k}) = \begin{pmatrix}
0 & \tilde{\Phi}'(\vec{k})_{00} \\
\tilde{\Phi}'(\vec{k})_{00} & 0
\end{pmatrix} \begin{pmatrix}
\tilde{\psi}_{A0}(\vec{k}) \\
\tilde{\psi}_{B0}(\vec{k})
\end{pmatrix} = - \sum_{a=1,2} \begin{pmatrix}
0 & \tilde{\Phi}'(\vec{k})_{0a} \\
\tilde{\Phi}'(\vec{k})_{0a} & 0
\end{pmatrix} \begin{pmatrix}
\tilde{\psi}_{Aa}(\vec{k}) \\
\tilde{\psi}_{Ba}(\vec{k})
\end{pmatrix},
\] (48)
the tight binding model is reduced to the following form to the second order in $\tilde{k}$:

$$
H_{\text{eff}} = \int \frac{d^2k}{(2\pi)^2} \tilde{\psi}^\dagger(\tilde{k})[H_1(\tilde{k}) + H_2(\tilde{k})] \tilde{\psi}(\tilde{k}),
$$

(49)

$$
\tilde{\psi}(\tilde{k}) = \begin{pmatrix} \tilde{\psi}_{A1}(\tilde{k}) & \tilde{\psi}_{A2}(\tilde{k}) & \tilde{\psi}_{B1}(\tilde{k}) & \tilde{\psi}_{B2}(\tilde{k}) \end{pmatrix}^T,
$$

(50)

$$
H_1(\tilde{k}) = v \left\{ k_1 (\tau_2 \otimes \sigma_1) + k_2 (\tau_2 \otimes \sigma_2) \right\},
$$

(51)

$$
H_2(\tilde{k}) = \frac{v^2}{3t} \left\{ 2(k_1^2 + k_2^2)(\tau_1 \otimes 1_{2\times 2}) + \frac{1}{2}(k_1^2 - k_2^2)(\tau_1 \otimes \sigma_1) - (k_1k_2)(\tau_1 \otimes \sigma_2) \right\}
$$

(52)

with $v = at/2$, where the former of tensor structure acts on sub-lattice space $I = A, B$ and the latter of tensor structure acts on flavor space $a = 1, 2$ in the above tensor product representations. Here the first term of Eq.(49) is Dirac Hamiltonian in momentum space, while the second term of Eq.(49) is a higher derivative term suppressed by the mass of $\psi_0$, which is negligible in the low energy region.

Close to the continuum limit, we can neglect higher derivative terms $H_2(\tilde{k})$ in Hamiltonian (49), and the effective Hamiltonian has following 4 global symmetries in this approximation:

$$
1_{2\times 2} \otimes 1_{2\times 2}, \tau_1 \otimes \sigma_3, \tau_2 \otimes 1_{2\times 2}, \tau_3 \otimes \sigma_3.
$$

(53)

Considering a Parity invariant mass term, which is invariant under the Parity transformation (which is exchange symmetry of $A \leftrightarrow B$ and $x \rightarrow -x$ but $\rho \rightarrow \rho$ in Figure 2),

$$
m \tilde{\psi}^\dagger(\tilde{k})(\tau_1 \otimes 1_{2\times 2}) \tilde{\psi}(\tilde{k}),
$$

(54)

two global symmetries, $1_{2\times 2} \otimes 1_{2\times 2}$, $\tau_1 \otimes \sigma_3$, are preserved, whereas $\tau_2 \otimes 1_{2\times 2}$, $\tau_3 \otimes \sigma_3$ are broken. We call the symmetry under global rotation with generators $\tau_2 \otimes 1_{2\times 2}$, $\tau_3 \otimes \sigma_3$ as "naive chiral symmetry", which forbid the Parity invariant mass term Eq.(54), up to the first order of $\tilde{k}$ (in Table 1).

However the higher derivative term, which is the second term in Eq.(49), violates "naive chiral symmetry" like Wilson fermion formulation. This fact seems that the mass term may be easily induced through quantum corrections when we introduce interactions between electrons. In general, symmetries at finite lattice spacing may be deformed by lattice artifact.

We consider a possibility of modified chiral symmetry which depends on the momentum and determine its form exactly in next section. We will find that there exists a chiral symmetry which is reduced to the above chiral symmetry $\tau_3 \otimes \sigma_3$ in the continuum limit.

Note that in Legendre formulation Lagrangian is described as

$$
\mathcal{L} = i\tilde{\psi}(t, \bar{x}) \left[ \partial_0 \gamma_0 - v \sum_{i=1,2} \gamma_i \partial_i \right] \psi(t, x)
$$

(55)
where $\bar{\psi} = \psi^\dagger \gamma_0$ and gamma matrices $\gamma_0$, $\gamma_1$, $\gamma_2$ are,

$$
\begin{align*}
\gamma_0 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
\gamma_1 &= \begin{pmatrix} -i\sigma_1 & 0 \\ 0 & i\sigma_1 \end{pmatrix}, \\
\gamma_2 &= \begin{pmatrix} -i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}
\end{align*}
$$

(56)

(in details see also appendix). Apparently, these gamma matrices $\gamma_0, \gamma_1, \gamma_2$ satisfy Clifford algebra $\{\gamma_\mu, \gamma_\nu\} = g_{\mu\nu}$, where $g_{\mu\nu}$ is a metric in 2+1 dimensional space-time. These gamma matrices are connected $\hat{\gamma}_\mu$ in section 2 by an appropriate unitary transformation.

| Global symmetry | preserved | broken |
|-----------------|-----------|--------|
| $1_2 \otimes 2_2$ | $\tau_3 \otimes \sigma_3$ | $\tau_2 \otimes 1_2 \otimes 2$ | $\tau_3 \otimes \sigma_3$ |

Table 1: Symmetry in Effective Theory to the mass term

5  Exact chiral symmetry

In this section we consider the exact chiral symmetry in position formulation of graphene model under leading order of tight binding approximation. We consider a modified chiral symmetry at finite lattice spacing involving the first and second derivatives defined in Eq.(9).

Here we take following ansatz for exact chiral symmetry of Hamiltonian (18) in position space,

$$
\delta \chi(\vec{x}) = i\theta \left[ 3(\tau_3 \otimes X)\chi(\vec{x}) + \frac{1}{2} \sum_\rho (\tau_3 \otimes Y_\rho)(\Delta_\rho \chi(\vec{x}) + 2\chi(\vec{x})) + \frac{1}{i} \sum_\rho (1 \otimes Z_\rho)(\nabla_\rho \chi(\vec{x})) \right],
$$

(57)

where $X, Y_\rho$, and $Z_\rho$ are $3 \times 3$ hermite matrices. Based on this ansatz, we look for the solution for the symmetry equation $\delta \mathcal{H} = 0$, and finally we determine its concrete form uniquely $^6$. An explicit calculation of $X, Y_\rho$, and $Z_\rho$ is shown in appendix $^3$ and here we show the result as follows:

$$
\delta \chi(\vec{x}) = i\theta \left[ 3(\tau_3 \otimes X)\chi(\vec{x}) + \frac{1}{2} \sum_\rho (\tau_3 \otimes Y_\rho)(\Delta_\rho \chi(\vec{x}) + 2\chi(\vec{x})) + \frac{1}{i} \sum_\rho (1 \otimes Z_\rho)(\nabla_\rho \chi(\vec{x})) \right]
$$

(58)

$^6$ Generally, there are two possibilities for $\hat{\Gamma}_5$ in Eq.(69), which is consistent with the results in section 4. One is $\hat{\Gamma}_5 = \tau_3 \otimes X + \mathcal{O}(\alpha)$, which is supposed above derivation, and the other is $\hat{\Gamma}_5 = \tau_2 \otimes X_2 + \mathcal{O}(\alpha)$, which might be consistent with naive chiral symmetry $\tau_2 \otimes 1_2 \otimes 2$ in effective theory. Thus, we consider both cases. However the latter is found not to satisfy the symmetry equation at the second order in momentum expansion.
with

\[
X = \begin{pmatrix}
0 & -i & i \\
-1 & 0 & -i \\
i & -1 & 0 \\
i & 0 & -i \\
0 & i & 0 \\
0 & 0 & 1 \\
i & 0 & 0 \\
i & 0 & -1 \\
0 & 0 & -1 \\
i & 0 & 0 \\
i & 0 & -i \\
0 & 0 & -i \\
i & 0 & 0 \\
i & 0 & -i
\end{pmatrix},
\]

(59)

\[
Y_0 = \begin{pmatrix}
0 & -i & i \\
i & 0 & 0 \\
-1 & 0 & 0 \\
-1 & 0 & 0 \\
i & 0 & -i \\
i & 0 & -i \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad Y_1 = \begin{pmatrix}
0 & -i & 0 \\
i & 0 & -i \\
0 & i & 0 \\
i & 0 & -i \\
0 & 0 & i \\
i & 0 & -i \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad Y_2 = \begin{pmatrix}
0 & 0 & i \\
0 & 0 & -i \\
0 & 0 & 0 \\
0 & 0 & -i \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

(60)

\[
Z_0 = \begin{pmatrix}
0 & -1 & 1 \\
-1 & 0 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad Z_1 = \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & -1 & 0 \\
1 & 0 & -1 \\
0 & 0 & -1 \\
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad Z_2 = \begin{pmatrix}
0 & 0 & 1 \\
0 & 0 & -1 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & -1 \\
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

(61)

If we take a continuum limit \( a \to 0 \), above chiral transformation becomes \( \delta \chi(\vec{x}) = 3i\theta X\chi(\vec{x}). \) Here, taking mass basis, \( X \) may be transformed to following form, except for an overall factor,

\[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & -1 & 0
\end{pmatrix}.
\]

(62)

Thus, the exact chiral symmetry corresponds to chiral symmetry in the continuum \( \tau_3 \otimes \sigma_3 \) in effective theory, which is consistent with the results in section 4.

### 6 Summary and discussion

In this paper we study how to construct Dirac fermion from honeycomb lattice in position space. In our formulation we make new labeling of fermion field in which the fundamental lattice is composed of the centers of hexagonal unit cells. The six sites in each unit hexagonal cell is reinterpreted as spin-flavor degrees of freedom.

Starting from the tight binding model, we find that the Hamiltonian is constructed by kinetic term and second derivative term of three flavor Dirac fermion in which one flavor has a mass of cutoff order and the other flavors are massless. In our formulation the structure of the Dirac point is simplified so that its uniqueness can be easily shown. We also explicitly show that there exist an exact chiral symmetry at finite lattice spacing, which protects the masslessness of the Dirac fermion, under the nearest neighbor interaction.

From the point of view in lattice gauge theory, the graphene model introduced in ref.[4] or in this paper seems analogous to the staggered fermion formulation [5]. In the staggered fermion formulation, there exists two representations of Dirac fermion with grassmann variables spread over hypercubic lattice. One is defined in momentum space [6] and the other is defined in position space [7]. In the former formulation the momentum space is divided
into $2^d$ regions (where the size of the Brillouin Zone (BZ) becomes half in each direction) and the staggered fermion field defined in these regions can be regarded as $2^{d/2}$ flavor Dirac fields. While, in the latter case, the staggered fermion defined in hypercubes which has $2^d$ corners is introduced and Dirac field with $2^d$ spin-flavor is defined by multi-product of Dirac gamma matrices on Grassmann variables. Comparing to the Graphene model suggested by Semenoff, in which Dirac fermion is defined as two excitations on different regions in BZ, it is very analogous to the staggered fermion in momentum space formulation[6]. On the other hand, our formulation is analogous to the position space formulation for staggered fermion found in ref.[7].

The formulation in position space easily extends toward the gauge interacting system and also provides the complementary ingredients for understanding of the connection to QED with 2+1 dimensional fermion brane [10, 11], Monte-Carlo simulation of non-relativistic action [12, 13] and honeycomb lattice simulation [14, 15]. Furthermore, since our formulation has manifest structure of flavor symmetry, the analytical study of dynamical nature of graphene such as the spontaneous symmetry breaking in this formulation will be comparable with lattice simulations.

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**A Model in Lagrange formulation**

If we add a mass term to the effective theory, Hamiltonian is written as follows;

$$
\mathcal{H} = \int \frac{d^2k}{(2\pi)^2} \tilde{\psi}^\dagger(\vec{k})[\alpha_1 k_1 + \alpha_2 k_2 + m\beta] \tilde{\psi}(\vec{k}),
$$

where

$$
\begin{align*}
\alpha_1 &= \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix}, \\
\alpha_2 &= \begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix}.
\end{align*}
$$

$\beta$ is a Hermitian matrix and we may take following choices;

$$
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

Here the first gives parity even mass term and the second gives parity odd mass term. However the parity odd mass term may be forbidden by parity, thus we choose the parity
even mass term here. Then transforming above Hamiltonian to Lagrangian in real space, we obtain following Dirac Lagrangian in configuration space.

\[
L = i\bar{\psi}(t, \vec{x}) \left[ \partial_0 + v \sum_{i=1,2} \alpha_i \frac{\partial}{\partial x_i} - m \beta \right] \psi(t, \vec{x})
\] (66)

\[
= i\bar{\psi}(t, \vec{x}) \left[ \partial_0 \gamma_0 - v \sum_{i=1,2} \gamma_i \frac{\partial}{\partial x_i} - m \right] \psi(t, \vec{x})
\] (67)

where \( \bar{\psi} = \psi^\dagger \beta \) and \( \gamma_0 = \beta, \gamma_1 = -\beta\alpha_1, \gamma_2 = -\beta\alpha_2 \). Evidently the gamma matrices \( \gamma_0, \gamma_1, \gamma_2 \) satisfy Clifford algebra \( \{ \gamma_\mu, \gamma_\nu \} = g_{\mu\nu} \), where \( g_{\mu\nu} \) is a metric in 2+1 dimensional space-time.

### B Explicit calculation of exact chiral symmetry

In order to determine \( X, Y, Z, \) we employ momentum representation of \( \chi(\vec{x}), \chi^\dagger(\vec{x}) \)

\[
\mathcal{H} = \int \frac{d^2k}{(2\pi)^2} \bar{\chi}(\vec{k}) \left[ (\tau_1 \otimes \Lambda) + \sum_\rho e^{ik_\rho (\tau_- \otimes \Gamma_\rho)} + \sum_\rho e^{-ik_\rho (\tau_+ \otimes \Gamma_\rho)} \right] \chi(\vec{k})
\] (68)

with \( \tau_\pm \equiv (\tau_1 \pm i\tau_2)/2 \) and \( \Lambda \equiv M - 1 \), and for chiral transformation \( \delta \bar{\chi}(\vec{k}) = i\theta \Gamma_5(\vec{k})\chi(\vec{k}) \)

\( \bar{\Gamma}_5(\vec{k}) \) is given as

\[
\bar{\Gamma}_5(\vec{k}) = (\tau_3 \otimes X) + \sum_\rho e^{ik_\rho \gamma_\rho} + \sum_\rho e^{-ik_\rho \gamma_\rho^\dagger},
\] (69)

with

\[
\gamma_\rho = \frac{\tau_3 + 1}{2} \otimes W_\rho^\dagger + \frac{\tau_3 - 1}{2} \otimes W_\rho.
\] (70)

Here, imposing \( [\bar{\mathcal{H}}(\vec{k}), \bar{\Gamma}_5(\vec{k})] = 0 \), we obtain following equations;

\[
\{ \Lambda, X \} + \sum_\rho (\Gamma_\rho W_\rho + W_\rho^\dagger \Gamma_\rho) = 0
\] (71)

\[
\{ \Gamma_\rho, X \} + \Lambda W_\rho^\dagger + W_\rho \Lambda = 0
\] (72)

\[
\Lambda W_\rho + W_\rho^\dagger \Lambda + \sum_{\sigma \neq \lambda(\sigma \neq \rho)} (\Gamma_\sigma W_\lambda^\dagger + W_\lambda \Gamma_\sigma) = 0
\] (73)

\[
\Gamma_\rho W_\rho^\dagger + W_\rho \Gamma_\rho = 0
\] (74)

\[
\Gamma_\rho W_\sigma + W_\sigma^\dagger \Gamma_\rho = 0 \quad (\rho \neq \sigma).
\] (75)

Solving these equation for \( X \) and \( W_\rho(\rho = 0, 1, 2) \), the solutions are found to be

\[
X = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix},
\] (76)

\[
W_0 = \begin{pmatrix} 0 & -i & i \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad W_1 = \begin{pmatrix} 0 & 0 & 0 \\ i & 0 & -i \\ 0 & 0 & 0 \end{pmatrix}, \quad W_2 = \begin{pmatrix} 0 & 0 & 0 \\ -i & i & 0 \end{pmatrix}.
\] (77)
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