Magnetoelectric response of the antiferromagnetic insulator phase in a three-dimensional correlated system with spin-orbit coupling

Akihiko Sekine and Kentaro Nomura

Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

E-mail: sekine@imr.tohoku.ac.jp

Abstract. We theoretically investigate the antiferromagnetic insulator phase in a three-dimensional correlated system with spin-orbit coupling, the Fu-Kane-Mele-Hubbard model at half-filling. We focus on the topological magnetoelectric effect which is described by the theta term. A low-energy effective Hamiltonian is derived in the antiferromagnetic insulator phase. Then with the use of a field-theoretical method, the theta term is derived as a consequence of the chiral anomaly.

1. Introduction

Topological phases of matter have attracted a great deal of attention recently. Three-dimensional (3D) topological insulators are one of such phases. They can be characterized by the topological magnetoelectric response described by the so-called theta term. The theta term is given by [1]

$$S_\theta = \int dt d^3x \frac{\theta e^2}{32\pi^2 \hbar c} \epsilon^{\mu\nu\rho\lambda} F_{\mu\nu} F_{\rho\lambda} = \int dt d^3x \frac{\theta e^2}{4\pi^2 \hbar c} \boldsymbol{E} \cdot \boldsymbol{B}, \tag{1}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ with A_μ being the electromagnetic four-potential. $\boldsymbol{E}$ and $\boldsymbol{B}$ are an electric field and magnetic field, respectively. From this action, the cross-correlated response of the electric polarization $\boldsymbol{P}$ and magnetization $\boldsymbol{M}$ is obtained as $\boldsymbol{P} = \theta e^2/(4\pi^2\hbar c)\boldsymbol{B}$ and $\boldsymbol{M} = \theta e^2/(4\pi^2\hbar c)\boldsymbol{E}$. In particle physics, the phenomenon described by the theta term is called the axion electrodynamics, since θ is considered as the field operator of an elementary particle, axion. In (time-reversal invariant) 3D topological insulators, the coefficient θ takes the quantized value $\theta = \pi$ (mod 2π), while $\theta = 0$ in normal insulators. However, it is known that the value of θ can be arbitrary between 0 and π in time-reversal symmetry broken systems [2].

The interplay of spin-orbit coupling and electron correlation has been studied intensively, in the search for novel phases and novel phenomena. One of the triggers is the discovery of a novel Mott insulating state in a $5d$ correlated electron system with spin-orbit coupling [3]. It should be noted that the emergence of topological phases such as quantum spin Hall insulator [4], topological Mott insulator [5], topological magnetic insulator [6], and Weyl semimetal [7] has been predicted theoretically. In this paper, we focus on the topological magnetoelectric response of the antiferromagnetic insulator phase (i.e., a time-reversal symmetry broken phase) in a 3D correlated system with spin-orbit coupling.

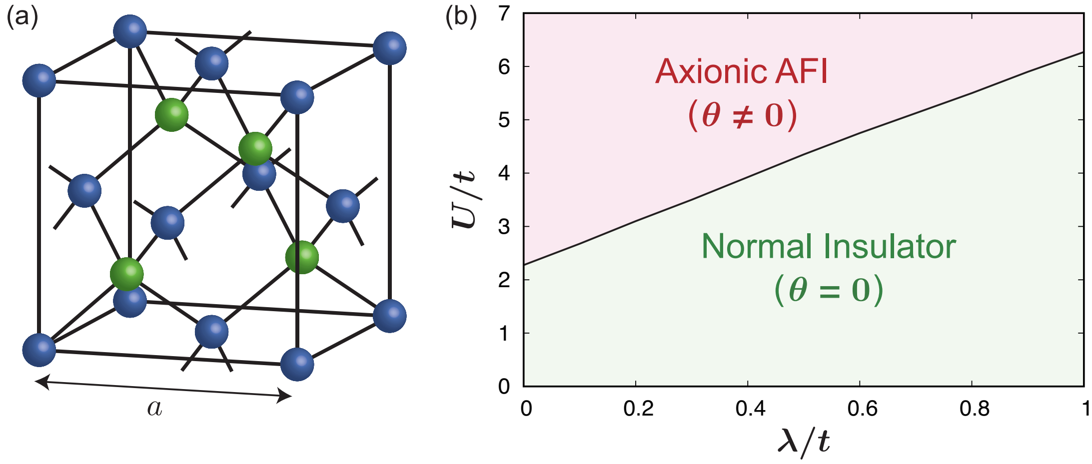

Figure 1. (a) A diamond lattice. Each sublattice (blue and green) forms a fcc lattice. (b) Mean-field phase diagram of the half-filled Fu-Kane-Mele-Hubbard model on a diamond lattice, with the antiferromagnetic ordering set to the [111] direction, in the case of $\delta t_1/t = -0.5$. In the antiferromagnetic insulator (AFI) phase, the value of θ becomes nonzero and, as a result, the topological magnetoelectric response arises.

2. Model and the mean-field phase diagram

The model we consider is the Fu-Kane-Mele-Hubbard model on a diamond lattice at half-filling. The lattice structure of a diamond lattice is shown in Fig. 1(a). The Hamiltonian of the system is given by

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + i\frac{4\lambda}{a^2} \sum_{\langle\langle i,j\rangle\rangle} c^\dagger_i \boldsymbol{\sigma}\cdot(\boldsymbol{d}^1_{ij}\times\boldsymbol{d}^2_{ij})c_j + U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{2}$$

where $c^\dagger_{i\sigma}$ is an electron creation operator at a site i with spin $\sigma(=\uparrow,\downarrow)$, $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$, and a is the lattice constant of the fcc lattice. $\boldsymbol{d}^1_{ij}$ and $\boldsymbol{d}^2_{ij}$ are the two nearest-neighbor bond vectors which connect two sites i and j of the same sublattice. $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices for the spin degree of freedom. The first through third terms of H represent nearest-neighbor hopping, next-nearest-neighbor spin dependent hopping (i.e. spin-orbit interaction), and on-site electron-electron interaction, respectively.

Let us express H_0, the non-interacting part of the Hamiltonian, in terms of the 4×4 matrices α_μ which satisfy the Clifford algebra $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}$. The diamond lattice consists of two sublattices (A and B), with each sublattice forming a fcc lattice. In such a case, it is convenient to define the basis as $c_{\boldsymbol{k}} \equiv [c_{\boldsymbol{k}A\uparrow}, c_{\boldsymbol{k}A\downarrow}, c_{\boldsymbol{k}B\uparrow}, c_{\boldsymbol{k}B\downarrow}]^T$ where the wave vector $\boldsymbol{k}$ is given by the points in the first Brillouin zone of the fcc lattice. Then the single-particle Hamiltonian $\mathcal{H}_0(\boldsymbol{k})$ $[H_0 \equiv \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}}\mathcal{H}_0(\boldsymbol{k})c_{\boldsymbol{k}}]$ is written as $\mathcal{H}_0(\boldsymbol{k}) = \sum_{\mu=1}^5 R_\mu(\boldsymbol{k})\alpha_\mu$, where the coefficients $R_\mu(\boldsymbol{k})$ are given by [8]

$$\begin{aligned}
R_1(\boldsymbol{k}) &= \lambda[\sin u_2 - \sin u_3 - \sin(u_2 - u_1) + \sin(u_3 - u_1)],\\
R_2(\boldsymbol{k}) &= \lambda[\sin u_3 - \sin u_1 - \sin(u_3 - u_2) + \sin(u_1 - u_2)],\\
R_3(\boldsymbol{k}) &= \lambda[\sin u_1 - \sin u_2 - \sin(u_1 - u_3) + \sin(u_2 - u_3)],\\
R_4(\boldsymbol{k}) &= t + \delta t_1 + t(\cos u_1 + \cos u_2 + \cos u_3),\\
R_5(\boldsymbol{k}) &= t(\sin u_1 + \sin u_2 + \sin u_3).
\end{aligned} \tag{3}$$

Journal of Physics: Conference Series **592** (2015) 012128 doi:10.1088/1742-6596/592/1/012128

Here $u_1 = \boldsymbol{k} \cdot \boldsymbol{a}_1$, $u_2 = \boldsymbol{k} \cdot \boldsymbol{a}_2$, and $u_3 = \boldsymbol{k} \cdot \boldsymbol{a}_3$ with $\boldsymbol{a}_1 = \frac{a}{2}(0,1,1)$, $\boldsymbol{a}_2 = \frac{a}{2}(1,0,1)$ and $\boldsymbol{a}_3 = \frac{a}{2}(1,1,0)$ being the primitive translation vectors. Note that we have introduced the lattice distortion along the [111] direction, which results in the modification of the hopping strength for the [111] direction as $t_{ij} = t + \delta t_1$ while $t_{ij} = t$ for the other three directions. The system becomes gapped due to nonzero δt_1, whereas the system is gapless when $\delta t_1 = 0$. When $0 < \delta t_1 < 2t$ ($\delta t_1 < 0$ or $\delta t_1 > 2t$), the system is identified as a topological insulator (normal insulator) [8]. In the following, we set $a = 1$.

Let us perform the mean-field approximation to the interaction term and derive the mean-field Hamiltonian of the system. At half-filling, spin-density wave (SDW) orderings are expected to develop when on-site interactions are strong. In our model, due to the spin-orbit interaction, the spin SU(2) symmetry is broken and the orientations of the spins are associated with the lattice structure. Hence we assume the antiferromagnetic ordering between the two sublattices in terms of the spherical coordinate (m, θ, φ):

$$\langle \boldsymbol{S}_{i'A} \rangle = -\langle \boldsymbol{S}_{i'B} \rangle = (m \sin\theta \cos\varphi, m \sin\theta \sin\varphi, m \cos\theta) \equiv m_1 \boldsymbol{e}_x + m_2 \boldsymbol{e}_y + m_3 \boldsymbol{e}_z, \tag{4}$$

where $\langle \boldsymbol{S}_{i'\mu} \rangle = \frac{1}{2} \langle c^\dagger_{i'\mu\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i'\mu\beta} \rangle$ ($\mu = A, B$) with i' denoting the i'-th unit cell. In the mean-field decoupling process, both the Hartree and Fock terms are taken into account. After a calculation, the mean-field Hamiltonian of the system is obtained as [9]

$$H_{\mathrm{MF}} = 2NUm^2 + \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} \mathcal{H}_{\mathrm{MF}}(\boldsymbol{k}) c_{\boldsymbol{k}}, \tag{5}$$

where $\mathcal{H}_{\mathrm{MF}}(\boldsymbol{k}) = \sum_{\mu=1}^{5} \tilde{R}_\mu(\boldsymbol{k}) \alpha_\mu$ with $\tilde{R}_1(\boldsymbol{k}) = R_1(\boldsymbol{k}) - Um_1$, $\tilde{R}_2(\boldsymbol{k}) = R_2(\boldsymbol{k}) - Um_2$, $\tilde{R}_3(\boldsymbol{k}) = R_3(\boldsymbol{k}) - Um_3$, $\tilde{R}_4(\boldsymbol{k}) = R_4(\boldsymbol{k})$, and $\tilde{R}_5(\boldsymbol{k}) = R_5(\boldsymbol{k})$. We have used the fact that $m_1^2 + m_2^2 + m_3^2 = m^2$. N is the number of the unit cells, and the wave vectors $\boldsymbol{k}$ take N points in the first Brillouin zone of the fcc lattice. From the mean-field Hamiltonian, we can readily obtain the free energy at zero temperature for the SDW instability:

$$F_{\mathrm{SDW}}(m, \theta, \varphi) = 2NUm^2 - 2 \sum_{\boldsymbol{k}} \sqrt{\sum\nolimits_{\mu=1}^{5} [\tilde{R}_\mu(\boldsymbol{k})]^2}. \tag{6}$$

The ground state is given by the stationary condition $\partial F_{\mathrm{SDW}}(m,\theta,\varphi)/\partial m = \partial F_{\mathrm{SDW}}(m,\theta,\varphi)/\partial \theta = \partial F_{\mathrm{SDW}}(m,\theta,\varphi)/\partial \varphi = 0$.

The phase diagram with antiferromagnetic ordering set to the [111] direction in the case of $\delta t_1/t = -0.5$ is shown in Fig. 1(b) as an example. Phase diagrams for other antiferromagnetic ordering directions and for the positive value of δt_1 are qualitatively same as Fig. 1(b). The transition from the normal insulator phase to the antiferromagnetic insulator phase is of the second order. We see from the phase diagram that the critical strength of the on-site interaction U_c becomes larger as the strength of the spin-orbit interaction λ becomes larger. Such a behavior can be understood from that the free energy (6) is characterized by the factor U/λ in $\tilde{R}_j(\boldsymbol{k})$ ($j = 1, 2, 3$). Namely, the strong spin-orbit interaction effectively makes the on-site interaction weaker. Similar results have been obtained in the Kane-Mele-Hubbard model, a 2D analog of our model [10, 11]. However, as is shown below, what is peculiar to the antiferromagnetic phase in the 3D Fu-Kane-Mele-Hubbard model is the emergence of the topological magnetoelectric response described by the theta term.

3. Low-energy effective Hamiltonian and the theta term in the antiferromagnetic insulator phase

In this section, we derive the theta term with the use of a field-theoretical method. To this end, first we need to derive the low-energy effective Hamiltonian in the antiferromagnetic insulator phase. In the following, we consider the general case given by the order parameter (4). In the non-interacting system with $\delta t_1 = 0$, it is known that the energy band touching occurs at the three X points where $X^x = (2\pi, 0, 0)$, $X^y = (0, 2\pi, 0)$ and $X^z = (0, 0, 2\pi)$, and that massless Dirac Hamiltonians are derived around these points [8]. Similarly when $\delta t_1 \neq 0$, massive Dirac Hamiltonians are obtained. That is, the low-energy effective model near the Fermi level is described by Dirac quasiparticles. We see that Dirac Hamiltonians can be obtained also in the antiferromagnetic phase, by expanding the mean-field single-particle Hamiltonian $\mathcal{H}_{\rm MF}(\boldsymbol{k})$ around the three $\tilde{X}$ points with $\boldsymbol{k} = \tilde{X} + \boldsymbol{q}$, and retaining the terms up to the order of $\boldsymbol{q}$:

$$\begin{aligned}
\mathcal{H}_{\rm MF}(\tilde{X}^x + \boldsymbol{q}) &= tq_x\alpha_5 + 2\lambda q_y\alpha_2 - 2\lambda q_z\alpha_3 + \delta t_1\alpha_4 - Um_1\alpha_1, \\
\mathcal{H}_{\rm MF}(\tilde{X}^y + \boldsymbol{q}) &= tq_y\alpha_5 + 2\lambda q_z\alpha_3 - 2\lambda q_x\alpha_1 + \delta t_1\alpha_4 - Um_2\alpha_2, \\
\mathcal{H}_{\rm MF}(\tilde{X}^z + \boldsymbol{q}) &= tq_z\alpha_5 + 2\lambda q_x\alpha_1 - 2\lambda q_y\alpha_2 + \delta t_1\alpha_4 - Um_3\alpha_3,
\end{aligned} \tag{7}$$

where $\tilde{X}^x = \left(2\pi, \frac{Um_2}{2\lambda}, -\frac{Um_3}{2\lambda}\right)$, $\tilde{X}^y = \left(-\frac{Um_1}{2\lambda}, 2\pi, \frac{Um_3}{2\lambda}\right)$, and $\tilde{X}^z = \left(\frac{Um_1}{2\lambda}, -\frac{Um_2}{2\lambda}, 2\pi\right)$. The condition $Um_f \ll 2\lambda$ ($f = 1, 2, 3$) is imposed. Here let us recall that the representation of α_μ is arbitrary as far as the Clifford algebra $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}$ is satisfied. Further the above three Dirac Hamiltonians are independent of each other. With the definition $\alpha_5 = \alpha_1\alpha_2\alpha_3\alpha_4$, relabeling of α_μ enables us to rewrite Eq. (7) as

$$\begin{aligned}
\mathcal{H}_{\rm MF}(\tilde{X}^x + \boldsymbol{q}) &= q_x\alpha_1 + q_y\alpha_2 + q_z\alpha_3 + \delta t_1\alpha_4 + Um_1\alpha_5, \\
\mathcal{H}_{\rm MF}(\tilde{X}^y + \boldsymbol{q}) &= q_x\alpha_1 + q_y\alpha_2 + q_z\alpha_3 + \delta t_1\alpha_4 + Um_2\alpha_5, \\
\mathcal{H}_{\rm MF}(\tilde{X}^z + \boldsymbol{q}) &= q_x\alpha_1 + q_y\alpha_2 + q_z\alpha_3 + \delta t_1\alpha_4 + Um_3\alpha_5,
\end{aligned} \tag{8}$$

where we have rescaled the momenta $\boldsymbol{q}$ around each $\tilde{X}$ point. These three equations are equivalent except for the α_5 terms. Namely, the low-energy effective model of the antiferromagnetic insulator phase is described by the Dirac fermions of *three flavors* characterized by the α_5 terms.

Then the Euclidean action of the Dirac fermions in the presence of an external electromagnetic field A_μ is given by

$$S_{\rm AFI} = \int d^4x \sum_{f=1,2,3} \bar{\psi}_f(x) \left[\gamma_\mu D_\mu - M_f e^{i\kappa_f\gamma_5}\right] \psi_f(x), \tag{9}$$

where $\psi_f(x)$ is a four-component spinor, $D_\mu = \partial_\mu + ieA_\mu$, $M_f = \sqrt{(\delta t_1)^2 + (Um_f)^2}$, $\cos\kappa_f = |\delta t_1|/M_f$, $\sin\kappa_f = Um_f/M_f$, and we have used the fact that $\alpha_4 = \gamma_0$, $\alpha_5 = -i\gamma_0\gamma_5$ and $\alpha_j = \gamma_0\gamma_j$ ($j = 1, 2, 3$). The subscript f denotes the flavor. Here we have considered the case of $\delta t_1 < 0$, namely the system is a normal insulator when $U = 0$. We employ the Fujikawa's method [12, 13] to derive the theta term from the above action. After applying the infinitesimal chiral transformation defined by

$$\psi_f \to \psi'_f = e^{-i\kappa_f d\phi\gamma_5/2}\psi_f, \quad \bar{\psi}_f \to \bar{\psi}'_f = \bar{\psi}_f e^{-i\kappa_f d\phi\gamma_5/2} \quad (d\phi \ll 1,\ \phi \in [0, 1]) \tag{10}$$

to the partition function $Z = \int \mathcal{D}[\psi, \bar{\psi}] e^{-S_{\rm AFI}[\psi,\bar{\psi}]}$ infinite times, we obtain $S_{\rm AFI} = S_{\rm NI} + S_\theta$ [9], where $S_{\rm NI}$ is the action which represents the normal insulator phase in our model and S_θ is the theta term:

$$S_{\rm NI} = \int d^4x \sum_f \bar{\psi}_f(x) \left[\gamma_\mu D_\mu - M_f\right] \psi_f(x), \qquad S_\theta = i \int d^4x \frac{(\sum_f \kappa_f)e^2}{32\pi^2\hbar c} \epsilon^{\mu\nu\rho\lambda} F_{\mu\nu} F_{\rho\lambda}. \tag{11}$$

From the theta term, the value of θ in the antiferromagnetic insulator phase is given by

$$\theta = \sum_{f=1,2,3} \kappa_f = \sum_{f=1,2,3} \tan^{-1}(Um_f/|\delta t_1|), \tag{12}$$

where the order parameter m_f is a function of U and λ. The region where $\theta \neq 0$ is shown in Fig. 1(b). As mentioned in the introduction, the emergence of the theta term results in the topological magnetoelectric response such that $\boldsymbol{P} = \theta e^2/(4\pi^2\hbar c)\boldsymbol{B}$ and $\boldsymbol{M} = \theta e^2/(4\pi^2\hbar c)\boldsymbol{E}$. Here note that the above expression of θ is valid when the condition $Um_f \ll 2\lambda$ is satisfied, i.e., it is valid near the phase boundary.

4. Discussions and Summary

So far we have obtained an analytical expression for θ in the antiferromagnetic insulator phase as a function of the on-site interaction strength U and the spin-orbit interaction strength λ. It is known that the value of θ can be arbitrary between 0 and π in time-reversal symmetry broken 3D systems, while $\theta = 0$ in normal insulators and $\theta = \pi$ in 3D topological insulators. The arbitrary value of θ means the time-reversal symmetry breaking of the system. Regardless of its value, nonzero value of θ distinguishes axionic antiferromagnetic insulators from trivial antiferromagnetic insulators. It should be noted that the theta term is derived only in odd spatial dimensions. In one dimension, from the theta term $S_{(1+1)D} = \int dtdx \frac{\theta}{2\pi} E$, the electric polarization $P_{1\mathrm{D}}$ is obtained as $P_{1\mathrm{D}} = \theta/(2\pi)$. Namely, the ground state is polarized.

We see from the low-energy effective Hamiltonian (8) that the antiferromagnetic phase of our model is characterized by the α_5 terms. Actually, the matrix α_5 breaks time-reversal symmetry (and spatial inversion symmetry). Further, from the definition of the chiral transformation (10), we see that the existence of the α_5 terms is essential to generate nonzero values of θ. The derivation of the low-energy effective Hamiltonian (8) is therefore crucial in this study.

Here let us briefly consider the case where the antiferromagnetic order parameter is fluctuating around the ground-state direction as $\boldsymbol{m}(\boldsymbol{x},t) = [m_1 + \delta m_1(\boldsymbol{x},t)]\boldsymbol{e}_x + [m_2 + \delta m_2(\boldsymbol{x},t)]\boldsymbol{e}_y + [m_3 + \delta m_3(\boldsymbol{x},t)]\boldsymbol{e}_z$. In such a case, it is easily shown from Eq. (12) that the deviation of the value of θ from the ground-state value is given by $\delta\theta(\boldsymbol{x},t) \approx U/|\delta t_1| \sum_f \delta m_f(\boldsymbol{x},t)$. This means that the dynamical axion field can be realized by the antiferromagnetic spin-wave excitation, which leads to the axionic polariton phenomenon [6]. As 3D correlated systems with spin-orbit coupling, for example, iridium oxides could be experimental candidates.

To summarize, we have studied theoretically the half-filled Fu-Kane-Mele-Hubbard model on a diamond lattice, focusing on the topological magnetoelectric response described by the theta term. We have obtained a mean-field phase diagram in the on-site interaction strength versus spin-orbit interaction strength plane. With the use of a field-theoretical method, the Fujikawa's method, the theta term was derived. The emergence of the topological magnetoelectric response in the antiferromagnetic insulator phase can be understood as a result of the interplay of spin-orbit coupling and electron correlation.

Acknowledgments

A.S. is supported by the JSPS Research Fellowship for Young Scientists. This work was supported by Grant-in-Aid for Scientific Research (No. 25103703, No. 26107505 and No. 26400308) from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

References

[1] Qi X-L, Hughes T L and Zhang S-C 2008 *Phys. Rev.* B **78** 195424
[2] Essin A M, Moore J E and Vanderbilt D 2009 *Phys. Rev. Lett.* **102** 146805
[3] Kim B J, Jin H, Moon S, Kim J-Y, Park B-G, Leem C, Yu J, Noh T, Kim C, Oh S-J, Park J-H, Durairaj V, Cao G and Rotenberg E 2008 *Phys. Rev. Lett.* **101** 076402

[4] Shitade A, Katsura H, Kuneš J, Qi X-L, Zhang S-C and Nagaosa N 2009 *Phys. Rev. Lett.* **102** 256403
[5] Pesin D and Balents L 2010 *Nat. Phys.* **6** 376
[6] Li R, Wang J, Qi X-L and Zhang S-C 2010 *Nat. Phys.* **6** 284
[7] Wan X, Turner A M, Vishwanath A and Savrasov S Y 2011 *Phys. Rev.* B **83** 205101
[8] Fu L and Kane C L 2007 *Phys. Rev.* B **76** 045302
[9] Sekine A and Nomura K 2014 *J. Phys. Soc. Jpn.* **83** 104709
[10] Rachel S and Le Hur K 2010 *Phys. Rev.* B **82** 075106
[11] Hohenadler M, Lang T C and Assaad F F 2011 *Phys. Rev. Lett.* **106** 100403
[12] Fujikawa K 1979 *Phys. Rev. Lett.* **42** 1195
[13] Fujikawa K 1980 *Phys. Rev.* D **21** 2848