Electric and magnetic fields tuned spin-polarized topological phases in two-dimensional ferromagnetic MnBi$_2$Te$_7$

Shi Xiao,$^{1, 2}$ Xiaoliang. Xiao,$^{1, 2}$ Fangyang Zhan,$^{1, 2}$ Jing Fan,$^3$ Xiaozhi Wu,$^{1, 2}$ and Rui Wang$^{1, 2, 3, 4, \dagger}$

$^1$Institute for Structure and Function and Department of Physics, Chongqing University, Chongqing 400044, P. R. China
$^2$Chongqing Key Laboratory for Strongly Coupled Physics, Chongqing 400044, P. R. China
$^3$Center for Computational Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, P. R. China
$^4$Center for Quantum Materials and Devices, Chongqing University, Chongqing 400044, P. R. China

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Over the past decades [1–4], the exploration of topological phases of matter has attracted intensive interest in condensed matter physics. Among various topological phases, one of the most important members is the time-reversal (TR) invariant topological insulator (TI) with a $	ext{Z}_2$ index, which was first predicted in two-dimensional (2D) graphene [5, 6] and HgTe quantum well [7], and experimentally confirmed soon in the latter [8]. The 2D TI with the $T$-symmetry is also termed as the quantum spin Hall (QSH) insulators. Later for a long time, the TR-symmetry is considered to be a prerequisite to QSH states. In fact, when the $T$-symmetry is absent, the combination of topology and magnetism can lead to more fruitful spin-polarized nontrivial phases, such as quantum anomalous Hall (QAH) effects [9–14], TR-symmetry broken QSH effects [15], topological magnetoelectric effects [16, 17], Majorana fermions [18–22], and magnetic Weyl fermions [23, 24]. Among these topological phenomena, the QAH effect with dissipationless chiral edges and quantized Hall conductance is one of the most fascinating topics.

The QAH effect was first been observed experimentally in magnetically doped TI thin films [9]. However, magnetic dopants require that the QAH effect only occurs in ultralow temperatures due to inhomogeneity of ferromagnetic order. Comparing with magnetically doped systems, an undoped stoichiometric material prefers to form ordered magnetic structures. Therefore, for purposes of practical application, there have been many theoretical proposals for realizing high-temperature QAH effects in intrinsically magnetic insulating systems [25–31]. But, unfortunately, the experimental confirmation of QAH effects in intrinsic magnetic materials has been relatively slow.

Recently, the van der Waals (vdW) Mn-Bi-Te superlattices MnBi$_2$Te$_4$/(Bi$_2$Te$_3$)$_n$ ($n = 0, 1, 2, 3, \ldots$) have guided significant advancements of QAH effects or other spin-polarized topological phases with intrinsic mechanism both in theories and experiments [11, 12, 32, 33]. The compound MnBi$_2$Te$_4$ (i.e., $n = 0$) is composed of Te-Bi-Te-Mn-Te-Bi-Te septuple layers, and compounds MnBi$_2$Te$_4$/(Bi$_2$Te$_3$)$_n$ ($n = 0, 1, 2, 3, \ldots$) are in essence $1 : n$ formalism of a MnBi$_2$Te$_4$ septuple layer and a Bi$_2$Te$_3$ quintuple layer. These layered compounds exhibit intralayer ferromagnetism and interlayer antiferromagnetism, resulting in their topological features dependent on odd or even numbers of layers [34–37]. Remarkably, the QAH effect up to 1.4 K without the aid of external magnetic fields has been observed in a five-septuple-layer of MnBi$_2$Te$_4$ [11]. Beyond MnBi$_2$Te$_4$, other vdW Mn-Bi-Te superlattices such as MnBi$_4$Te$_7$ and MnBi$_6$Te$_{10}$ (i.e., $n = 1, 2$) also currently stimulate extensive interest to realize various spin-polarized topological phases [12, 38–46].

As is well known, applying an external field such as electric or magnetic fields is widely used to not only tune topological states but also facilitate their observations in experiments [11, 15, 47–56]. For instance, the observed temperature of QAH effects in the five-septuple-layer MnBi$_2$Te$_4$ film under a small magnetic field can remarkably be increased up to 6.5 K [11], and the combi-
nation of a magnetic field and back gate voltage can give rise to a high-Chern-number QAH effect in ten-septuple-layer MnBi$_2$Te$_4$ film [57] or drive a phase transition from the axion insulating phase to the QAH phase in the six-septuple-layer MnBi$_2$Te$_4$ film [56, 58] at relatively high temperatures. Therefore, a theoretical study of spin-polarized topological phases in Mn-Bi-Te systems tuned by external electric or magnetic fields is desirable.

In this work, based on first-principles calculations and topological analysis, we identify that the MnBi$_4$Te$_7$ monolayer with a ferromagnetic (FM) groundstate exhibits the TR-symmetry broken QSH effect, which possesses a quantized spin Hall conductance associated with the nonzero spin Chern number. The nontrivial band gap of the TR-symmetry broken QSH phase can be considerably enlarged by applying an external positive electric fields perpendicular to the MnBi$_4$Te$_7$ atomic plane. Furthermore, using the Wannier-function-based tight-binding (WFTB) approach, we reveal that a topological phase transition from the TR-symmetry broken QSH phase to the QAH phase occurs with the increase of Zeeman exchange energy of magnetic fields. Finally, we present a phase diagram to fully understand cooperative effects of electric and magnetic fields.

II. COMPUTATIONAL METHODS

To investigate electronic properties of monolayer MnBi$_4$Te$_7$, we carried out first-principles calculations as implemented in Vienna ab initio simulation package [59, 60] based on the density-functional theory (DFT) [61, 62]. The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) formalism was employed to describe the exchange-correlation functional [63]. The electron-ion interaction was treated by projector-augmented-wave potentials [64]. The cutoff energy of the plane wave basis was set to 500 eV, and the Brillouin zone was sampled with a 12×12×1 Monkhorst-Pack grid [65]. Since the correlation effects of Mn 3$d$ electrons, we employed the GGA+U method [66] and set the $U = 5$ eV [67, 68]. The forces on each atom were relaxed to be less than 0.001 eV/Å. A 15 Å vacuum layer along the $z$ direction was used to avoid the interaction between neighboring layers. The effects of applying external electric fields normal to the MnBi$_4$Te$_7$ monolayer was directly including in DFT calculations. The topological properties were revealed by constructing a WFTB Hamiltonian based on maximally localized Wannier functions methods combining DFT calculations [69–71]. The WFTB Hamiltonian with Mn $d$, Bi $p$, and Te $p$ orbitals can well reproduce the DFT electronic band structures including spin-orbital coupling (SOC) effects in the range of $E_F \pm 2$ eV [see Fig. S1]. The topological edge states such as the local density of states (LDOS) were computed using WANNIERTOOLS package based on the iterative Greens method [72, 73].

To reveal the electronic properties under magnetic fields, we consider an Zeeman exchange energy

$$H_Z = \tilde{g} \mu_B (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B},$$

in which $\tilde{g}$, $\mu_B$, $\mathbf{L}$, and $\mathbf{S}$ represent the effective $g$-factor, Bohr magneton, orbital angular momentum, and spin angular momentum, respectively. As a result, the total Hamiltonian can be expressed as $H_T = H_{SOC}(\mathbf{k}) + H_Z$, in which the WFTB Hamiltonian $H_{SOC}(\mathbf{k})$ in the presence of SOC is

$$H_{SOC}(\mathbf{k}) = \sum_{\alpha\beta} \langle \psi_{k,\alpha} | H_{SOC} | \psi_{k,\beta} \rangle$$

$$= \sum_{\alpha\beta} \sum_{\mathbf{R}} e^{i \mathbf{k} \cdot \mathbf{R}} t_{\alpha\beta}(\mathbf{R} - 0)$$

with

$$t_{\alpha\beta}(\mathbf{R} - 0) = \langle 0 + s_\alpha | H_{SOC} | \mathbf{R} + s_\beta \rangle.$$  \hspace{1cm} (3)

Here, $| \psi_k \rangle$ are Bloch states over the $\mathbf{k}$ space, $\mathbf{R}$ is the Bravais lattice vector, and $t_{\alpha\beta}(\mathbf{R} - 0)$ are the hopping parameters from orbital $\beta$ at site $s_\beta$ in the home cell at $\mathbf{R} = 0$ to orbital $\alpha$ at site $s_\alpha$ in the unit cell located at $\mathbf{R}$. Note that we here ignore the Peierls phase in the hopping parameters $t_{\alpha\beta}$ or Landau levels. This approach is reliable and effective for studying the magnetic field induced evolution of topological states [74, 75].
As shown in Fig. 1, the MnBi$_4$Te$_7$ monolayer can be considered as the Bi$_2$Te$_3$/MnBi$_2$Te$_4$ heterostructure with the hexagonal symmetry, i.e., a Bi$_2$Te$_3$ quintuple layer on top of a MnBi$_2$Te$_4$ septuple layer. The hexagonal unit cell is denoted by two basic vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, which satisfy $|\mathbf{a}_1| = |\mathbf{a}_2| = a$ [see Fig. 1(b)]. The optimized in-plane lattice constants are 4.37 Å and 4.43 Å for MnBi$_2$Te$_4$ and Bi$_2$Te$_3$, respectively, and thus the small difference ($\sim 1.35\%$) of their lattice constants only leads to a tiny mismatch between two layers. The optimized equilibrium distance between Bi$_2$Te$_3$ and MnBi$_2$Te$_4$ layers is 2.68 Å, indicating that there is a considerable interlayer hybridization between Bi$_2$Te$_3$ and MnBi$_2$Te$_4$ layers. As shown in Fig. 1(c), the differential charge density indicates that electrons transfer from the MnBi$_2$Te$_4$ layer to the Bi$_2$Te$_3$ layer, forming a built-in electric field in MnBi$_2$Te$_4$. In this case, outer shell electrons of Bi and Te atoms near the interface would suffer a charge redistribution to maintain the charge balance. As a result, though their interlayer coupling [see Fig. 1(c)] can facilitate the electron transfer from the MnBi$_2$Te$_4$ layer to the Bi$_2$Te$_3$ layer, forming a built-in electric field in MnBi$_2$Te$_4$. The system would undergo a topological phase transition with band gap closing and then reopening if gradually turning on SOC. The band gap of MnBi$_4$Te$_7$ as a function of the SOC strength. The band gap of MnBi$_4$Te$_7$ can be tuned by applying external electric fields (or changing interlayer distance). At the critical gapless point, the bands touch at the Fermi level. Since the built-in electric field induced by interlayer hybridization and charge transfer is present between Bi$_2$Te$_3$ and MnBi$_2$Te$_4$ layers, the nontrivial band gap of MnBi$_4$Te$_7$ can be tuned by applying external electric fields (or changing interlayer distance). As shown in Fig. 2(c), we schematically illustrate the band gap as a function of the electric field $E$ (or the variation of interlayer distance $\delta d$).
direction along $z$ axis is normal to the MnBi$_4$Te$_7$ plane; meanwhile, the variation of interlayer distance $\delta d$ is defined as $\delta d = d - d_0$ with the optimized equilibrium distance $d_0$. As expected, it is found that a positive electric field can effectively enhance the interlayer hybridization and thus enlarge the nontrivial band gap. As shown in Fig. S2 in the SM [78], we can see that the band inversion at $\Gamma$ is still preserved when the electric field strength increases to 0.2 V/A. In this case, the nontrivial band gap can be considerable up to $\sim 102$ meV [see Fig. 2(e)]. That is to say, applying external electric fields or changing interlayer distance in the physical regime does not change the nontrivial band topology of MnBi$_4$Te$_7$.

For a FM nontrivial system, there are usually two distinct topological phases with bulk band gaps [15]. The one is the TR-symmetry broken QSH insulator with nonzero spin Chern number $C^*$, and the other is the QAH insulator with nonzero Chern number $C$. The Chern number $C$ and spin-Chern number $C^*$ are respectively defined as $C = C_\uparrow + C_\downarrow$ and $C^* = C_\uparrow - C_\downarrow$, where $C_\uparrow$ and $C_\downarrow$ are the spin-dependent Chern numbers of spin-up and spin-down sectors, respectively. To determine the topological phase of MnBi$_4$Te$_7$ monolayer, we calculate the evolution of Wannier charge centers (WCC) for the full closed plane of $k_z = 0$ using the Wilson loop method [79]. As shown in Fig. 3(a), the calculated results indicate that the referenced line can always cross the WCC line even times, i.e., the Chern number $C = 0$. Hence, the MnBi$_4$Te$_7$ monolayer does not belong to the QAH insulator but may be the TR-symmetry broken QSH insulator. To further confirm this, we calculated the spin Hall conductance $\sigma^s_{xy}$ using the Kubo formula [80],

$$\sigma^s_{xy} = \frac{e}{\hbar} \int \frac{dk_x dk_y}{(2\pi)^2} \Omega^s_k,$$

$$\Omega^s_k = 2\text{Im} \sum_{m \neq n} \frac{\langle \psi_{nk}|j^s_x|\psi_{nk}\rangle \langle \psi_{nk}|v_y|\psi_{nk}\rangle}{(E_m - E_n)^2},$$

where $v_i$ ($i = x, y$) is the velocity operator, $E_{nk}$ is the eigenvalue of the Bloch functions $\psi_{nk}$, and $j^s_x = 1/2\{s_z, v_x\}$ denotes a spin current operator in the $x$ direction. From Eq. (4), we calculate the spin Hall conductance $\sigma^s_{xy}$ with WFTB Hamiltonian using WANNIER90 package [70]. The calculated $\sigma^s_{xy}$ of MnBi$_4$Te$_7$ as a function of the Fermi level is plotted in Fig. 3(b). We can see that the value of $\sigma^s_{xy}$ is quantized to $C^*$ as $C^* = -2$ inside the nontrivial band gap, which is contributed from the spin Berry curvature $\Omega^s_k$ in the momentum space. As shown in Fig. 3(c), we can see that both the positive and negative $\Omega^s_k$, which are with respective to the three-fold rotational symmetry, clearly diverges near the $\Gamma$ point, uncovering the nontrivial band topology of MnBi$_4$Te$_7$. We show the calculated LDOS of a semi-infinite of MnBi$_4$Te$_7$ in Fig. 3(d). Distinct from the gapless Dirac cone of TR-symmetry protected QSH phase, the Dirac cone formed from two edge states is slightly gapped [see the inset of Fig. 3(d)], demonstrating the presence of TR-symmetry broken QSH phase in MnBi$_4$Te$_7$ [15].

Figure 3: (a) The evolution of WCC of MnBi$_4$Te$_7$ in the full closed plane of $k_z = 0$. The referenced line is denoted by the red dashed line. (b) The spin Hall conductance $\sigma^s_{xy}$ of MnBi$_4$Te$_7$ as a function of the Fermi level. Inside the band gap, the spin Hall conductance $\sigma^s_{xy}$ is quantized to $C^*$ with $C^* = 2$. (c) The Berry curvature distribution of MnBi$_4$Te$_7$. The first BZ is marked by the white lines. (d) The calculated LDOS of a semi-infinite of MnBi$_4$Te$_7$. The inset shows that the Dirac cone formed from two edge states is slightly gapped.

Compared with the TR-symmetry broken QSH phase, the QAH phase with chiral edge states and quantized anomalous Hall conductance is more interesting. The previous investigation demonstrated that the competition between the QAH and TR-symmetry broken QSH phases was dependent on the relation of Rashba SOC and Zeeman exchange fields [15]. On the one hand, applying external electric fields (or changing interlayer distance) can potentially affect the Rashba SOC and then tune the nontrivial band gap of TR-symmetry broken QSH phase [see Fig. 2(e)]. On the other hand, an external magnetic field can effectively enhance the magnetic exchange energy in intrinsically magnetic material. Therefore, we next study the evolution of topological properties in MnBi$_4$Te$_7$ under external magnetic fields.

By applying an external magnetic fields $\mathbf{B}$ normal to the MnBi$_4$Te$_7$ plane along the $z$ axis, one can find that the band gap first closes and then reopens (see Fig. S3 in the SM [78]), implying the occurrence of a topological phase transition. The critical gapless point at the $K$ valley occurs at the Zeeman exchange energy of 170 meV. Beyond the threshold of Zeeman exchange energy, we calculate the evolution of WCC for the full closed plane of $k_z = 0$ as shown in Fig. 4(a). The referenced line can always cross the WCC line one times, implying the presence of QAH phase with $C = 1$. To fur-
Figure 4: (a) The evolution of WCC of MnBi$_4$Te$_7$ in the full closed plane of $k_z = 0$. The referenced line is denoted by the red dashed line. Here, the perpendicular electric field strength and Zeeman exchange energy are respectively set to -0.2 V/Å and 130 meV. In this case the QAH phase is present. (b) The intrinsic Hall conductance $\sigma_{xy}$ of MnBi$_4$Te$_7$ as a function of the Fermi level. Inside the bang gap, $\sigma_{xy}$ is quantized to $e^2/h$. (c) The calculated LDOS exhibits chiral edge states of QAH phase. (d) The phase diagram as functions of the Zeeman exchange energy and electric field strength.

ther confirm that the QAH phase is indeed present in MnBi$_4$Te$_7$, we also calculate the intrinsic Hall conductance $\sigma_{xy}$ [see Fig. 4(b)]. It is found that the quantized plateau of $C^- = 1$ inside the nontrivial band gap is clearly visible. The semi-infinite LDOS of MnBi$_4$Te$_7$ is plotted in Fig. 4(c), exhibiting one nontrivial chiral edge state connecting the valence and conduction bands. As depicted in Fig. 2(e), a reverse electric field can effectively weaken the Rashba SOC and thus reduce the nontrivial band gap of TR-symmetry broken QSH phase, which is favourable to realize topological phase transition from the TR-symmetry broken QSH phase to the QAH phase. Therefore, to fully understand electric and magnetic fields tuned spin-polarized topological properties of MnBi$_4$Te$_7$, we calculate a phase diagram as functions of the Zeeman exchange energy and electric field strength [see Fig. 4(d)]. We can see that the electric field can effectively reduce the threshold of Zeeman exchange energy, thus facilitating to experimentally achieve the QAH phase in MnBi$_4$Te$_7$.

IV. SUMMARY

In summary, based on first-principles calculations and the WFTB approach, we uncover manipulated spin-polarized topological phases manipulated by the external electric and magnetic fields in the MnBi$_4$Te$_7$ monolayer with a FM groundstate. The external electric and magnetic fields respectively affect the Rashba SOC and magnetic exchange energy, and thus tune the nontrivial band gap and induce the topological phase transition. In the absence of external fields, the MnBi$_4$Te$_7$ monolayer possesses the TR-symmetry broken QSH phase with the spin Chern number $C^s = -2$. The nontrivial band gap of TR-symmetry broken QSH phase is highly tunable. Furthermore, the increase of Zeemann exchange energy of magnetic fields leads to a topological phase transition from the TR-symmetry broken QSH phase to the QAH phase with Chern number $C = 1$. Our work can promote to further understand cooperative effects of electric and magnetic fields on spin-polarized topological phases. Besides, this findings can also stimulate potential applications of nontrivially topological spintronics in intensive Mn-Bi-Te systems.

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[1] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[2] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[4] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[5] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[6] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[7] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).
[8] M. K. S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).
[9] C.-Z. Chang, J. Zhang, X. Feng, J. Shen, Z. Zhang, M. Guo, K. Li, Y. Ou, P. Wei, L.-L. Wang, Z.-Q. Ji, Y. Feng, S. Ji, X. Chen, J. Jia, X. Dai, Z. Fang, S.-C. Zhang, K. He, Y. Wang, L. Lu, X.-C. Ma, and Q.-K. Xue, Science 340, 167 (2013).
[10] R. Yu, W. Zhang, H.-J. Zhang, S.-C. Zhang, X. Dai, and
[53] C. Liu, Y. Wang, M. Yang, J. Mao, H. Li, Y. Li, J. Li, H. Zhu, J. Wang, L. Li, Y. Wu, Y. Xu, J. Zhang, and Y. Wang, Nat. Commun. 12, 4647 (2021).
[54] J. Böttcher, C. Tutschku, and E. M. Hankiewicz, Phys. Rev. B 101, 195433 (2020).
[55] H. Li, L. Sheng, and D. Y. Xing, Phys. Rev. B 85, 045118 (2012).
[56] J. Li, C. Wang, Z. Zhang, B.-L. Gu, W. Duan, and Y. Xu, Phys. Rev. B 100, 121103 (2019).
[57] C. Liu, Y. Wang, H. Li, Y. Wu, Y. Li, J. Li, K. He, Y. Xu, J. Zhang, and Y. Wang, Nat. Mater. 19, 522 (2020).
[58] J. Ge, Y. Liu, J. Li, H. Li, T. Luo, Y. Wu, Y. Xu, and J. Wang, Natl. Sci. Rev. 7, 1280 (2020).
[59] G. Kresse and J. Furthmüller, Comput. Mater. Sci. 6, 15 (1996).
[60] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
[61] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
[62] W. Kohn and L. Sham, Phys. Rev. 140, A1133 (1965).
[63] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[64] P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
[65] H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).
[66] A. I. Liechtenstein, V. I. Anisimov, and J. Zaanen, Phys. Rev. B 52, R5467 (1995).
[67] S. V. Eremeev, V. N. Men’shov, V. V. Tugushev, P. M. Echenique, and E. V. Chulkov, Phys. Rev. B 88, 144430 (2013).
[68] Y. S. Hou, J. W. Kim, and R. Q. Wu, Phys. Rev. B 101, 121401 (2020).
[69] N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997).
[70] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, Comput. Phys. Commun. 178, 685 (2008).
[71] J. Qiao, J. Zhou, Z. Yuan, and W. Zhao, Phys. Rev. B 98, 214402 (2018).
[72] Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov, Comput. Phys. Commun. 224, 405 (2018).
[73] M. P. L. Sancho, J. M. L. Sancho, J. M. L. Sancho, and J. Rubio, J. Phys. F: Met. Phys. 15, 851 (1985).
[74] J. W. Villanova and K. Park, Phys. Rev. B 98, 075123 (2018).
[75] Y. Choi, J. W. Villanova, and K. Park, Phys. Rev. B 101, 035105 (2020).
[76] S. Du, P. Tang, J. Li, Z. Lin, Y. Xu, W. Duan, and A. Rubio, Phys. Rev. Research 2, 022025 (2020).
[77] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nat. Phys. 5, 438 (2009).
[78] See Supplemental Material for the computational details.
[79] R. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, Phys. Rev. B 84, 075119 (2011).
[80] A. Crépieux and P. Bruno, Phys. Rev. B 64, 014416 (2001).