Nexus networks in carbon honeycombs

Yuanping Chen, Yuee Xie, Yan Gao, Po-Yao Chang, Shengbai Zhang, and David Vanderbilt

1 School of Physics and Optoelectronics, Xiangtan University, Xiangtan, 411105 Hunan, China
2 Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA
3 Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

(Received 22 February 2018; published 27 April 2018)

Nexus metals represent a new type of topological material in which nodal lines merge at nexus points. Here we propose novel networks in nexus systems through intertwining between nexus fermions and additional nodal lines. These nexus networks can be realized in recently synthesized carbon honeycomb materials. In these carbon honeycombs, we demonstrate a phase transition between a nexus network and a system with triply degenerate points and additional nodal lines. The Landau level spectra show unusual magnetic transport properties in the nexus networks. Our results pave the way toward realizations of new topological materials with novel transport properties beyond standard Weyl/Dirac semimetals.

DOI: 10.1103/PhysRevMaterials.2.044205

I. INTRODUCTION

The recent discovery of topological metals and semimetals offers new opportunities for observing elementary excitations in the condensed matter world that are not found in particle physics [1–7]. For examples, zero-dimensional nodal points with multiple degeneracy can be stabilized by crystalline symmetries [8–17] and one-dimensional objects such as Dirac and Weyl nodal lines can also exist in crystals [18–25]. These zero- and one-dimensional gapless excitations have no analog in elementary particle physics.

One interesting scenario for gapless excitation is the combined structure of nodal points and lines. In the presence of three mirror planes related by a threefold rotation and an additional mirror plane perpendicular to the rotation axis, two triple points (TPs) connected by a nodal line can be stabilized along the rotation axis [26–30]. By breaking the perpendicular mirror symmetry, this nodal line can split into four topological nodal lines, three of which reside on three mirrors planes while the last one remains on the rotation axis, as shown in Fig. 1(a). In this case, the TPs are referred to as nexus points (NPs), which can be seen as merging points of multiple nodal lines [31–35]. This transition has been predicted in several candidate materials [32–35]. New topological phenomena and transport properties created by nexus fermions have been proposed, such as unusual topological surface states [32], transport anomalies, and topological Lifshitz transitions [35].

Here we propose that the NP phase can further evolve into novel network structures. These networks originate from the original NP phase interacting with additional nodal lines protected by the mirror symmetry, as shown by the orange lines in Fig. 1(b). Because crossings between topological nodal lines are not allowed in the absence of any special symmetry constraint, anticrossing nodal lines are formed as shown in Fig. 1(c). As a result, nodal lines reconnect and the NPs become the intersection points of anticrossing nodal lines, as shown in Fig. 1(d). Considering that the system has three mirror planes, the NPs and the connecting nodal lines form a three-dimensional (3D) network in the full momentum space. We refer to this as a nexus network.

We propose that these nexus networks can be realized in carbon honeycombs (CHCs). Carbon honeycombs have recently been synthesized, although further refinement of the structure appears highly desirable [36]. We have identified two types of topological networks that can form in the carbon honeycombs. The first type is a nexus network in which the NPs are connected by nodal lines through two kinds of connectivities: a standard connectivity and a winding connectivity (we will define these later). The second type consists of TPs with additional nodal lines (ANLs), referred to as a TP-ANL network. These two types of networks correspond to different crystal symmetries. Therefore, the transition between these two networks can be induced by changing the corresponding crystal symmetries. In addition, we show that the Landau level (LL) spectrum can reveal the exotic magnetic transport properties of these two networks.

II. ATOMIC STRUCTURE OF A CHC AND COMPUTATIONAL METHOD

The atomic structure for a CHC is shown in Fig. 2(a), where carbon atoms form a 3D honeycomb structure. The atoms can be classified according to their characteristic orbital hybridization: $sp^2$ for carbon C1 and $sp^3$ for carbon C2. The C1 atoms can be further subdivided into two subgroups, as shown by the green and blue atoms, forming zigzag chains lying in mirror planes that intersect along the threefold axis [see Fig. 2(b)]. One can increase the width of the chains, corresponding to $n = 1$ in Fig. 2(a), to form wider CHC-$n$ nanoribbons with $n > 1$. The primitive cell of CHC-1 is shown...
in Fig. 2(b). The C2 atoms, on the other hand, form $sp^3$-bonded carbon dimers. In the absence of the dimerization, however, the honeycomb contains only $sp^2$-bonded carbon, as shown in Fig. 2(c), which will be termed CHC-1′ to distinguish it from CHC-1.

According to a space-group analysis, CHC-$n$ can be divided into two types. When $n$ is odd, the space group is $P3m1$ with a threefold rotational symmetry along $z$ and three mirror planes parallel to $z$. When $n$ is even, the space group is $P6_3/mmc$ with a sixfold screw rotational symmetry along $z$, a mirror plane $M_z$ normal to $z$, and three mirror and three glide planes parallel to $z$. Note that CHC-1′ also has the space group $P6_3/mmc$. Detailed structural parameters for the structures can be found in Table S1 in the Supplemental Information [37].

Our first-principles calculations were based on density functional theory (DFT) within the Perdew-Burke-Ernzerhof approximation for the exchange-correlation energy [38]. The core-valence interactions were described by the projector augmented-wave potentials, as implemented in the VASP code [39–41]. Plane waves with a kinetic energy cutoff of 600 eV were used as the basis set. The atomic positions were optimized via the conjugate gradient method, in which the energy convergence criterion between two consecutive steps was set at $10^{-6}$ eV. The maximum allowed force on the atoms is $10^{-3}$ eV/Å. A $9 \times 9 \times 15$ $k$-point mesh was used for the BZ integration of CHC-1 (or $1 \times 1 \times 2$ supercell of CHC-1′).

III. BAND STRUCTURE AND TOPOLOGICAL NETWORKS

Figure 3(a) shows the band structure of CHC-1 along $k_z$ ($\Gamma$-A), indicating that the carbon structure is metallic. There is a point $\alpha$ ($E = 0.50 \text{ eV}$, $k_z = 0.07\pi/c$, and $c = 4.83 \text{ Å}$ is the lattice constant along the $z$ axis) at which the black and green bands cross. Due to the negligibly small spin-orbit coupling strength in carbon, spin is neglected and the electrons are treated as spinless. In this context, the green band is doubly degenerate while the black band is nondegenerate. Therefore, the point $\alpha$ is a TP where three bands $m − 1$, $m$, and $m + 1$ cross ($m = 33$ here). Another TP is located at $k_z = −0.07\pi/c$ because of the structural inversion symmetry.

In a $k_y$-$k_z$ plane containing one TP, the TP appears as a crossing point of a Weyl cone and a flat energy band; however, in a $k_x$-$k_z$ (or $k_y$-$k_z$) plane containing both TPs, the two TPs are connected by a nodal line which is intersected by a cone and a tilted energy surface along $k_z$ (see Fig. S1 in [37]). The nodal line corresponds to the green band in Fig. 3(a), in which the solid and dotted parts represent degeneracy between bands $m − 1$ and $m$ and bands $m$ and $m + 1$, respectively. An examination clearly indicates that the TPs are also connected by other nodal lines on the three mirror planes $k_y = 0, \pm \sqrt{3}k_z$. Figure 3(d) exhibits the nodal lines for bands $m$ and $m + 1$ on the mirror plane $k_z = 0$, while Fig. 3(e) exhibits those for bands $m − 1$ and $m$. The two blue circles correspond to the TPs. As can be seen from Fig. 3(d), the two TPs are connected by a straight line and a curved line, both of which pass through the high-symmetry point A. The straight line corresponds to the dashed...
two ANLs coexist. It should be noted that to clearly show the nodal lines in (d)–(f), different scales of

\[ k_x, k_z \]

and \( k'_x, k'_z \) full first BZ of CHC-1

\[ m \]

equal to zero, that is, nodal lines. (e) Same as (d) but between bands shows a winding connectivity between two NPs. The blue circles correspond to the NPs, while the red lines represent the energy difference and \( m \) of the nexus network including NPs and nodal lines in the full first BZ. The solid and dotted lines correspond to nodal lines for bands \( m \) (blue circle) is a TP, as a result of band crossing between the double-degenerate (green) and nondegenerate (black) bands. (b) Schematic view of the nexus network including NPs and nodal lines in the full first BZ. The solid and dotted lines correspond to nodal lines for bands, while the red lines represent the energy difference equal to zero, that is, nodal lines. (c) Same as (d) but between bands \( m - 1 \) and \( m \), which shows a winding connectivity between two NPs. (f) Contour plots of energy difference between bands \( m - 1 \) and \( m \) on the mirror plane \( k_z = 0 \) for the structure CHC-1, which shows a standard connectivity between two NPs. The blue circles correspond to the NPs, while the red lines represent the energy difference close to the \( k_z \) axis, while those in the latter extend through the full BZ. It illustrates that this is a standard nexus phase like that in Fig. 1(a) and thus the TPs are in fact NPs connected by four nodal lines. Each mirror plane has a curved nodal line, while the three mirror planes share a straight line. We refer to this form of connection as a winding connectivity. The solid lines in Fig. 3(b) and \( k_z \) are in units of \( \pi / a \) and \( \pi / c \) (\( a \) and \( c \) are lattice constants), respectively.

By comparing the standard connectivity and winding connectivity, one can find that the nodal lines in the former remain close to the \( k_z \) axis, while those in the latter extend through the full BZ. Therefore, the nexus network may be easier to observe experimentally than the standard NP phase, because it extends the regions in which the topological elements can be found.

When the dimerization is removed, the CHC-1 structure evolves into CHC-1′, whose primitive cell is half that of CHC-1 as shown in Fig. 2(c). For comparison, the band structure for a \( 1 \times 1 \times 2 \) supercell of CHC-1′ is calculated. The results indicate that it is a TP-ANL metal, where TPs and ANLs coexist in momentum space. Figure 3(f) shows the nodal lines for bands \( m - 1 \) and \( m \) on the \( k_z = 0 \) mirror plane. Two TPs are located at \( k_z = \pm 0.07\pi / 2c' \) (\( c' \) is the lattice constant of CHC-1′) and they are connected by a straight nodal line. In addition, there are two nodal lines along \( k_z \). Because the structure has a sixfold screw symmetry, the other two mirror planes \( k_z = \pm \sqrt{3k_z} \) and three glide planes \( k_z = 0, \pm \sqrt{3k_z} \) have the same nodal line distributions as for the \( k_z = 0 \) plane. Figure 3(e) presents the whole topological network in the BZ. The ANLs cross at some points on the \( k_z \) axis other than at the TPs.
IV. TOPOLOGICAL PHASES BASED ON THE TIGHT-BINDING MODEL

We analyze the topological networks [see Figs. 3(b) and 3(c)] from a tight-binding model, which is designed to mimic the DFT band structure near the Fermi level. The bands of CHC-1 near the Fermi level are mainly contributed by $\pi$ orbitals on the sp$^2$-hybridized C1 atoms [see Fig. S1(b) in [37]]. Therefore, it is convenient to describe the carbon honeycomb by a tight-binding model

$$H = \sum_{\langle i,j \rangle} \sum_{\mu} t_{ij} e^{-ik \cdot d_{ij}^\mu},$$

where $i,j \in \{1,2,\ldots,12\}$ label the twelve C1 atoms, $d_{ij}^\mu$ is the displacement vector directed from atoms $j$ to $i$, $t_{ij}$ is the hopping energy between atoms $i$ and $j$, and $\mu$ runs over all lattice sites under translation. For $t_{ij}$, we include hoppings $t_0$ between atoms in the zigzag chains and hoppings $t_1 \sim t_5$ between the zigzag chains [see Figs. 2(a) and 2(b)].

To reveal the effect of structural symmetry on the electronic properties, we first consider the $1 \times 1 \times 2$ supercell of CHC-1'. It has space group $P6_3/mmc$, which includes a sixfold screw rotational symmetry along $z$, a mirror plane $M_z$ normal to $z$, and three mirror planes and three glide planes parallel to $z$. If we omit its C2 atoms, its electronic properties can also be described by Eq. (1). Due to the high symmetry, the values of $t_0 \sim t_5$ are simpler. Two subcases are considered according to $t_2$. When $t_2 = 0$, the tight-binding model represents a simple TP phase, in which two TPs are connected by a nodal line along $k_z$. Figure 4(a) shows the phase on one mirror plane $k_y = 0$. A further calculation indicates that each point on the nodal line is a crossing point of quadratic bands on the $k_x$-$k_y$ plane [the bands along $k_x$ are shown in Fig. 4(a1)]. The quadratic crossing leads to a trivial Berry phase of $2\pi$, which was computed for a closed loop around the crossing point. That is, the two TPs are connected by a Z$_2$-trivial line. When $t_2 \neq 0$, a TP-ANL phase like that of Fig. 3(c) is generated. In each mirror/glide plane, as shown in Fig. 4(b), two (orange) ANLs are now presented. Figure 4(b1) illustrates that each point on these ANLs is a crossing point of linear bands, leading to a nontrivial Berry phase of $\pi$. The crossing between the trivial green line and nontrivial orange lines is allowed because of protection by the structural symmetry. Following the evolution from Figs. 4(a) to 4(b), one can find that the parameter $t_2$ induces the ANLs on the mirror and glide planes.
FIG. 5. Extended TP-ANL phase and nexus network and LLs based on the \( \mathbf{k} \cdot \mathbf{p} \) model in Eq. (2) \([\beta \text{ is replaced by } \beta + \gamma \cos(\delta k_z)]\). (a) A TP-ANL phase in which a TP phase and four ANLs coexist \((\alpha = 0, \gamma = 0.5, \text{and } \delta = 4)\). (b) Nexus network evolved from (a) \((\alpha = 0.1, \gamma = 0.5, \text{and } \delta = 4)\). (c) The LLs for the TP-ANL phase in Fig. 4(b) \((\alpha = 0)\). (d) The LLs for the nexus network in Fig. 4(d) \((\alpha = 0.5)\). (e) and (f) The LLs for the TP-ANL phase in Fig. 5(a) and the nexus network in Fig. 5(b), respectively. The other parameters are \(A_1 = 1, B_1 = -1, A_2 = -1, B_2 = 1, D = 1, C_1 = C_2 = 0, \beta = -1, \text{and the magnetic field } B = 0.03\). Here \(k_x \text{ and } k_z \) are in units of \(\pi/a\) and \(\pi/c\), respectively.

We then consider the structure CHC-1. The dimers decrease the structural symmetry, which leads to the elimination of the three glide planes and the horizontal mirror plane \(M_z\) in CHC-1\(^\prime\). Atomic bond lengths of the structure become complicated and thus the values of \(t_0 \sim t_5\) become complicated. Two other subcases are now considered. When \(t_2 = 0\), the tight-binding model produces a standard NP phase. Figure 4(c) shows the nodal line structure on one mirror plane \(k_y = 0\). Comparing Figs. 4(a) and 4(c), one can see that the reduction of the symmetry causes the trivial nodal line in the TP phase to split into two nontrivial lines in the NP phase. This splitting originates from the fact that the quadratic points in Fig. 4(a1) split into two nodal points in Fig. 4(c1).

When \(t_2 \neq 0\), the novel nexus network in Fig. 3(d) is reproduced. Figure 4(d) shows the network on one mirror plane \(k_y = 0\). The two NPs are connected by standard connectivity for bands \(m\) and \(m + 1\), while they are connected by winding connectivity for bands \(m - 1\) and \(m\). The formation of the nexus network originates from the interactions between the standard NP phase and the ANLs. In the case of \(t_2 \neq 0\), the NP phase in Fig. 4(c) will overlap with the ANLs, which seems like Fig. 1(b). A crossing of two nontrivial lines is not generally allowed if there is no special symmetry to protect the crossing [42]. The nodal lines at the crossing point will split into two anticrossing lines, as shown in Fig. 1(c). As a consequence, the nodal lines in Fig. 1(b) evolve to adopt the structure shown in Fig. 1(d) or 4(d). (Detailed information about the tight-binding model is presented in [37].)

V. THE \( \mathbf{k} \cdot \mathbf{p} \) MODEL AND LANDAU LEVELS

Constrained by the symmetry groups and the time-reversal symmetry for spinless systems, one obtains a \( \mathbf{k} \cdot \mathbf{p} \) model around the \(\Gamma\) point

\[
H(k) = \begin{bmatrix}
A_1 k_z^2 + B_1 \cos k_z + C_1 & \alpha k_+ \sin k_z + \beta k_z^2 & D k_- \\
\alpha k_- \sin k_z + \beta k_z^2 & A_1 k_z^2 + B_1 \cos k_z + C_1 & -D k_+ \\
D k_+ & -D k_- & A_2 k_z^2 + B_2 \cos k_z + C_2
\end{bmatrix},
\]

where \(k_\pm = k_x \pm ik_y\), \(k_z^2 = k_x^2 + k_y^2\), and \(A_{1,2}, B_{1,2}, C_{1,2}, D\), \(\alpha\), and \(\beta\) are real constants. When \(\alpha = 0\), this model describes the topological phases in CHC-1\(^\prime\) with sixfold rotational symmetry. When \(\alpha \neq 0\), it describes those in CHC-1 because the
\[ ak_s \sin k_z \] term decreases the symmetry to threefold rotational symmetry. For the phases in CHC-1’, the \( \mathbf{k} \cdot \mathbf{p} \) model with \( \beta = 0 \) and \( \beta \neq 0 \) corresponds to the TP phase in Fig. 4(a) and TP-ANL phase in Fig. 4(b), respectively. Therefore, the effect of the \( \beta k_z^3 \) term is to generate ANLs on the mirror/glide planes. For the phases in CHC-1, Eq. (2) with \( \beta = 0 \) and \( \beta \neq 0 \) describes a standard NP phase as in Fig. 4(c) and a nexus network as in Fig. 4(d), respectively. Therefore, the effect of the \( \alpha k_s \sin k_z \) term is to split the trivial line in the TP phase. This further shows that the nexus network (\( \alpha \neq 0 \) and \( \beta \neq 0 \)) results from the interactions between the standard NP phase and the ANLs.

The reason to develop a \( \mathbf{k} \cdot \mathbf{p} \) model here is not only because such a generic model can reproduce the nexus network of CHC-1 (see Fig. S3 in [37]), but more importantly it depicts a more complete picture of the often-complicated nexus networks, which may not exist in the CHCs but may exist in other materials. For example, if \( \beta \) in Eq. (2) is replaced by \( \beta + \gamma \cos(\delta k_z) \), the different \( \gamma \) and \( \delta \) will generate rich TP-ANL phases and nexus networks (see Fig. S4 in [37]). Figure 5(a) presents a TP-ANL network that includes four ANLs in each mirror/glide plane, while Fig. 5(b) presents the corresponding nexus network that results when the TPs transition to NPs.

Based on Eq. (2), we calculate the LLs for the TP-ANL and nexus networks. As shown in Figs. 4(c)–4(f), besides the gapped LLs away from the Fermi level, there are gapless chiral LLs across the Fermi level. As mentioned above, the straight nodal line connecting TPs or NPs along \( k_z \) is intersected by a Weyl cone and a tilted energy surface. The gapped LLs are related to the cone, while the gapless chiral LLs originate from the tilted energy surface. Different behaviors of the chiral LLs come from different shapes of energy surfaces. For example, at the mirror plane \( k_y = 0 \), the eigenvalue of the tilted surface is

\[
E_1 = (A_1 + \beta) k_z^2 + \alpha k_z \sin k_z + B_1 \cos k_z + C_1. \tag{3}
\]

For the TP-ANL phases (\( \alpha = 0 \)), when \( A_1 = -\beta \), \( E_1 \) is a constant for a certain \( k_z \). This means that the energy surface is completely flat along the direction normal to \( k_z \). In this case, the chiral LLs collapse to one LL, as shown in Fig. 5(c). For the nexus network (\( \alpha \neq 0 \)), if \( A_1 = -\beta \), the chiral LLs become degenerate when \( k_z = 0, \pm \pi \), while remaining split at other \( k_z \), as shown in Fig. 5(d). Because of the structural threefold symmetry, the splitting LLs have threefold degeneracy.

For the complicated systems in Figs. 5(a) and 5(b), the chiral LLs become exotic. Figures 5(e) and 5(f) show their LLs, respectively. In Fig. 5(e), the chiral LLs form a standing-wave shape, with the wave nodes located at \( k_z = \pm \frac{\pi}{2} n \) for odd \( n \). This is because, when \( \gamma \cos(\delta k_z) = 0 \), the equation for the energy surface in this case becomes identical to Eq. (3). This constraint leads to \( k_z = \pm \frac{\pi}{2} n \) for the parameters given in Figs. 5(a) and 5(b) (\( \delta = 1 \)). Therefore, degenerate LLs appear at \( k_z = \pm \frac{\pi}{2} n \) for the TP-ANL phase (\( \alpha = 0 \)). For the nexus phase in Fig. 5(b), the chiral LLs split because \( \alpha \neq 0 \), as shown in Fig. 5(f). These exotic LLs not only exhibit identifying characteristics of the different topological phases, but also provide novel magnetic transport properties.

VI. DISCUSSION

The space group of CHC-\( n \) with even \( n \) is \( P6_3/mmc \), similar to that of CHC-1’. Therefore, TP-ANL phases exist in CHC-\( n \) (\( n = 2, 4, \ldots \)). Moreover, with the increase of \( n \), there exist fourfold-degenerate nodal points located between the TPs, which result in ANLs (see Fig. S5 in [37]). The structures CHC-\( n \) with odd \( n \) belong to the space group \( P\overline{3}m\overline{1} \) and all of them have nexus networks like CHC-1. Although the experiment in Ref. [36] reported that both periodic and random CHC structures have been obtained, these topological phases maybe are not easy to be observed in the recent samples because the crystal quality needs further improvement. We hope more experiments can be carried out to validate and extend our findings.

The topological classification of the nexus networks is different from that of standard NP phase. The nodal lines in the latter can be continuously contracted to a straight line. Those in the nexus networks, however, wind around the entire BZ torus and thus are not contractible. Mathematically, the BZ is topologically equivalent to a three-dimensional torus \( T^3 \). The connecting lines on \( T^3 \) can be classified under its fundamental homotopy group \( Z^3 \) [43], labeled by three integers, each indicating the number of times the loop winds around one of the three directions \( k_x, k_y, \) and \( k_z \). In this sense, the standard TP phase in Fig. 4(a) and standard NP phase in Fig. 4(c) belong to the trivial class with \( Z^3 = (0,0,0) \). However, the TP-ANL phases in Figs. 4(b) and 5(a) can be characterized as \( Z^3 = (1,0,0) \), and the nexus networks in Figs. 4(d) and 5(b) can be characterized as \( Z^3 = (2,0,0) \).

Nexus networks originate from the interactions between the standard NP phase and additional nodal lines. This creates the opportunity to propose and search for complex novel topological phases based on simpler topological elements. For example, the interactions between nodal lines/rings may lead to 3D nodal line networks [44] and the coexistence of multipoloid (threefold, fourfold, sixfold, and eightfold) degenerate points and nodal lines may generate more complicated new 3D networks. The new topological networks not only introduce emergent particles and novel concepts, but also create new topological phenomena and transport behaviors.

ACKNOWLEDGMENTS

We thank Damien West for useful discussions. Y.C. and Y.X. were supported by the National Natural Science Foundation of China (Grants No. 11474243 and No. 51376005). P.-Y.C. was supported by the Rutgers Center for Materials Theory. S.Z. were supported by the National Natural Science Foundation of China (Grants No. 11474243 and No. 51376005). D.V. was supported by the NSF Grant No. DMR-1408838.


[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevMaterials.2.044205 for describing the tight-binding model and the k · p model for CHC-1, the parameters for the two models, the DFT band structures of CHC-1 and CHC-2, the tight-binding band structure of CHC-1, the topological phases induced by the k · p model, and the structural parameters of CHC-1, CHC-2, and CHC-1'.

[42] For example, in the condition of time-reversal and inversion symmetry, we consider a Hamiltonian:

$$H(k) = f_0(k)\sigma_0 + f_1(k)\sigma_1 + f_3(k)\sigma_3,$$

where $k = (k_x, k_y, k_z)$ and $\sigma_0$, $\sigma_1$, and $\sigma_3$ are identity, first Pauli, and third Pauli matrices, respectively. The restrictions $f_1(k) = 0$ and $f_3(k) = 0$ apply two constrictions so the touchings are of dimension 1. Many choices for $f_1(k)$ and $f_3(k)$ are possible to generate two nodal lines. However, to allow the crossing of two lines, we must find a point $k_0$ satisfying $f_1(k_0) = 0$, $f_3(k_0) = 0$, and $\nabla f_1(k) = cf_3(k)$ ($c$ is a constant).
