Noncoplanar magnetic orders, in which spins align neither in a line nor on a plane, often lead to new low-energy excitations and/or topologically nontrivial states. In particular, triple-$Q$ magnetic orders, which are characterized by three different ordering wave vectors, have drawn much interest. A skyrmion lattice, found, e.g., in the A phase of MnSi [1], is a typical example of the triple-$Q$ orders, stabilized by competition between ferromagnetic and Dzyaloshinskii-Moriya interactions. Another example is found in geometrically frustrated lattices, which gives rise to a topological (Chern) insulator and associated quantum anomalous Hall effect: for instance, on kagome [2], distorted face-centered-cubic (FCC) [3], and triangular lattices [4–6].

In the present study, we investigate how a triple-$Q$ magnetic order affects the single-particle spectrum of itinerant electrons on a simple cubic lattice. We reveal that the spectrum exhibits a peculiar linear dispersion: namely, a triple-$Q$ magnetic order induces three-dimensional (3D) massless Dirac electrons. Furthermore, we show that such a Dirac electronic state in a triple-$Q$ order on a cubic lattice induces three-dimensional massless Dirac electrons. Furthermore, we show that such a Dirac electronic state in a triple-$Q$ order on a cubic lattice induces three-dimensional massless Dirac electrons. One is the emergence of surface states. Weyl electrons were recently proposed for an iridium pyrochlore oxide Y$_2$Ir$_2$O$_7$ [12]. Our result offers yet another example of Weyl electrons. Another interesting property is the emergence of surface states. Even without lifting the degeneracy of the Dirac electrons, our triple-$Q$ state exhibits peculiar gapless surface states with Fermi “arcs”.

FIG. 1. (color online). (a) Schematic picture of the noncoplanar four-sublattice triple-$Q$ order on a cubic lattice. Each spin points along the local [111] directions. A-D denote the four sublattices, respectively. (b) Energy dispersion of the Hamiltonian in Eq. (3) at $\Delta = 2t$, shown along the symmetric lines in the magnetic Brillouin zone displayed in (c), by connecting $\Gamma = (0,0,0)$, $N = (\pi/2, \pi/2, 0)$, $P = (\pi/2, \pi/2, \pi/2)$, and $H = (\pi,0,0)$. 3D massless Dirac points appear at the $P$ point, corresponding to $1/4$ and $3/4$ fillings.

This indicates that multiple-$Q$ orders exploit the possibility of engineering Dirac electrons by relaxing the symmetry constraints [8, 11].

In this Letter, we also clarify peculiar properties of the 3D massless Dirac electrons. One is the emergence of Weyl electrons in applied magnetic field. Our Dirac state is, at least, doubly degenerate. The degeneracy is lifted by applying magnetic field without gap opening, and the Dirac electronic state splits into a pair of Weyl states. Weyl electrons were recently proposed for an iridium pyrochlore oxide Y$_2$Ir$_2$O$_7$ [12]. Our result offers yet another example of Weyl electrons. Another interesting property is the emergence of surface states. Even without lifting the degeneracy of the Dirac electrons, our triple-$Q$ state exhibits peculiar gapless surface states with Fermi “arcs”.

Let us begin with explaining how a triple-$Q$ magnetic order induces 3D massless Dirac electrons. We con-
sider noninteracting electrons locally coupled to a triple-
Q magnetic order on the cubic lattice set by spins

$$S_i = m[\cos(Q_1 \cdot r_i) + \cos(Q_2 \cdot r_i) + \cos(Q_3 \cdot r_i)].$$

Here, $m$ is the triple-Q magnetic order parameter and $r_i$ is
the position vector of the site $i$ on the cubic lattice with
the lattice constant $a = 1$; $Q_1 = (\pi, 0, \pi)$, $Q_2 = (0, \pi, \pi)$,
$Q_3 = (\pi, \pi, 0)$ represent the wave vectors characterizing
the triple-Q state. $S_i$ has a noncoplanar four-sublattice
structure in the real space, as schematically shown in
Fig. 1(a). The Hamiltonian reads

$$H = \sum_{k, \sigma} \epsilon_k c_{k \sigma}^\dagger c_{k \sigma} + \frac{Jm}{2} \sum_{k, \sigma, \sigma', \eta} \epsilon_k \sigma \sigma' \sigma'' c_{k \sigma}^\dagger c_{k + Q_{\eta} \sigma''},$$

where $\epsilon_k (c_{k \sigma})$ is the creation (annihilation) operator of
a conduction electron with spin $\sigma$ at wave vector $k$.
The first term represents the kinetic energy of conduction
electrons and $\epsilon_k$ is the energy dispersion for free electrons
on the cubic lattice, $\epsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z)$. The
second term describes the coupling to triple-Q magnetic
order with the coupling constant $J$ ($\sigma$ is the Pauli
matrix and $\eta = 1, 2, 3$). In the four-sublattice representa-
tion, the Hamiltonian is divided into two irreducible parts

$$H = c_{l}^\dagger \tilde{H} c_l + c_{II}^\dagger \tilde{H} c_{II},$$

where

$$\tilde{H} = \begin{pmatrix} \epsilon_k & \Delta & -i\Delta & \Delta \\ \Delta & \epsilon_{k+Q_1} & -i\Delta & -\Delta \\ -i\Delta & -\Delta & \epsilon_{k+Q_2} & \Delta \\ \Delta & -i\Delta & \Delta & \epsilon_{k+Q_3} \end{pmatrix}.$$  

Here, $c_{l}^\dagger = (c_{k \uparrow}, c_{k+Q_1 \uparrow}, c_{k+Q_2 \uparrow}, c_{k+Q_3 \uparrow})$, $c_{II}^\dagger = (c_{k \downarrow}, -c_{k+Q_1 \downarrow}, -c_{k+Q_2 \downarrow}, c_{k+Q_3 \downarrow})$, and $\Delta = Jm/2$. We note
that this Hamiltonian is formally the same as that for
the four-sublattice triple-Q order on the triangular lattice [3].

The energy dispersion of the Hamiltonian in Eq. (3) is
shown in Fig. 1(b) at $\Delta = 2t$. Here, all the bands are
doubly degenerate; the degeneracy comes from the fact
that $c_l$ and $c_{II}$ are related by a combination of lattice
translation and spin rotation, which leaves $H$ unchanged.
In Fig. 1(b), notable features are found near the P
point, i.e., $k \simeq (\pi/2, \pi/2, \pi/2)$. There, the band dispersions
are linearly dependent on $k$ and cross with each other at
the P point, resulting in 3D cone-like structures. This is
a signature of 3D massless Dirac electrons appearing at
1/4 and 3/4 fillings of electrons.

The emergence of 3D massless Dirac electrons is
explicitly shown by a low-energy Hamiltonian near the P
point. Expanding the reduced Hamiltonian in Eq. (4)
around the P point and performing the unitary transfor-
mations, we obtain the low-energy effective Hamiltonian
up to the first order in $t/\Delta$ as

$$\tilde{H}_\pm = \pm \sqrt{3} \Delta \sigma_0 \pm \frac{2}{\sqrt{3}} t (\kappa_x \sigma_3 + \kappa_y \sigma_1 + \kappa_z \sigma_2),$$

where $\sigma_0$ is the $2 \times 2$ identity matrix and $\kappa$ is the trans-
formed wave vector measured from the P point. This
Hamiltonian constitutes a set of four-component Dirac
Hamiltonian $\tilde{H}_\pm = \tilde{H}_\pm \otimes I_{2 \times 2}$ that describes the 3D
massless Dirac electrons with a linear dispersion in all
the three directions of $\kappa$. The four-component Dirac
electrons are not chiral, as there is no unitary matrix which
anticommutes with the low-energy Hamiltonian. Such
a non-chiral 3D massless Dirac state cannot be turned
into an AIII topological insulator [16] by opening a gap,
though it is expected in 3D magnetically ordered phases.

Meanwhile, the twofold degeneracy in Eqs. (3) and (5)
is lifted by an external magnetic field. By adding the Zeeman
term proportional to $\sum_{k} (\epsilon_{k\uparrow} c_{k\uparrow} - \epsilon_{k\downarrow} c_{k\downarrow})$, the
degenerate Dirac point is split into two, and they are shifted
to the opposite directions along the $k_z$ axis. The resultant
nondegenerate nodes accommodate Weyl electrons,
which are robust against any perturbations respecting
the symmetry of the system. This gives an example of
Weyl electrons on the unfrustrated lattice, distinct from
those on a frustrated pyrochlore lattice [15].

Thus far, we simply assumed the noncoplanar triple-
Q magnetic order and discussed the resultant electronic
state. Now, we examine when and how the triple-Q state
is realized. We here consider one of the fundamental
models for d- and f-electron compounds, a periodic An-
derson model on the cubic lattice. The Hamiltonian is
given by

$$H = -t \sum_{(i,j), \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) - t_f \sum_{(i,j), \sigma} (f_{i\sigma}^\dagger f_{j\sigma} + H.c.)$$

$$- V \sum_{i, \sigma} (c_{i\sigma}^\dagger f_{i\sigma} + H.c.) + \frac{U}{2} \sum_{i, \sigma} n_{i\sigma}^f n_{i\sigma}^f$$

where $f_{i\sigma}^\dagger (f_{i\sigma})$ is the creation (annihilation) operator of
“localized” $f$ electrons with spin $\sigma$ at site $i$, and $n_{i\sigma}^f = f_{i\sigma}^\dagger f_{i\sigma}$. The first (second) term represents the kinetic
energy of conduction $c$ (“localized”) $f$ electrons, the third
term the on-site $c$-$f$ hybridization, the fourth term the
on-site Coulomb interaction for $f$ electrons, and the fifth
term the atomic energy of $f$ electrons. The sum of $(i,j)$
is taken over the nearest-neighbor sites on the cubic lattice.
Hereafter, we take $t = 1$ as an energy unit. We focus on a
commensurate filling, $n = (1/N) \sum_{i, \sigma} (c_{i\sigma}^\dagger c_{i\sigma} + f_{i\sigma}^\dagger f_{i\sigma}) = 3/2$, where $N$ is the total number of sites [17]. Note
that this corresponds to the 1/4-filling case in Eq. (2) when
the $f$ level is singly occupied to form a localized moment
at each site in the large $U$ limit.

In order to determine the ground state of the model in
Eq. (6), we employ the standard Hartree-Fock approx-
imation for the Coulomb $U$ term, which preserves the
SU(2) symmetry of the system. In the calculations, we
adopt the $2 \times 2 \times 2$-site unit cell, as shown in Fig. 1(a).
We also check the stability of the dominant phases by
using the $4 \times 4 \times 4$-site unit cell.
FIG. 2. (color online). Ground-state phase diagram of the periodic Anderson model [Eq. (6)] at 3/2 filling obtained by the mean-field calculations. $E_0$ and $t_f$ are taken at $-4$ and $0.2$, respectively. Schematic pictures of the ordering patterns in $f$ electrons are also shown. The sizes of circles reflect local electron densities, and the arrows represent local spin moments. AF, Ferro, Ferri, and CO stand for antiferromagnetic, ferromagnetic, ferrimagnetic, and charge-ordered states, respectively. Single-$Q$ corresponds to $Q = (\pi, 0, \pi)$, double-$Q$ $(0, \pi, \pi)$, $(\pi, 0, \pi)$, and triple-$Q$ $(\pi, \pi, 0)$, $(0, \pi, \pi)$, $(\pi, 0, \pi)$. C-double-$Q$ and other MO represent the canted double-$Q$ and other magnetically ordered states, respectively. In the triple-$Q$ CO phase, each charge-rich site has a small magnetic moment and its direction is antiparallel (parallel) to that at the diagonal charge-poor site in the region below (above) the dashed line.

Figure 2 shows the ground-state phase diagram obtained by the mean-field calculations. Schematic pictures of magnetic and charge states for $f$ electrons are shown in the bottom panel of Fig. 2. The result shows that various magnetic and CO states emerge in between the Néel-type collinear AF state in the $U \gg V$ region and the nonmagnetic (NM) Fermi liquid state in the large $V$ region. This indicates that the model in Eq. (6) has many instabilities which preempt the quantum critical point between AF and NM phases in the so-called Doniach phase diagram [18].

One of the dominant instabilities is a triple-$Q$ state, in which the spin configuration is equivalent to that in Eq. (1) [Fig. (1a)]. The result strongly suggests that the triple-$Q$ state is indeed stabilized in the microscopic model. Similar triple-$Q$ states were observed in intermetallic dysprosium compounds [19], and their origin is attributed to strong magnetic anisotropy along the local [111] directions. We note that our triple-$Q$ state is further stabilized by including such magnetic anisotropy.

Other dominant instabilities are the CO insulators accompanied by charge density modulation with wave vector $(\pi, \pi, \pi)$. A similar CO instability was discussed by the strong-coupling expansion [20] as well as numerical calculations [21–23] for the Kondo lattice model. In addition, a ferromagnetic CO was discussed in the periodic Anderson model [24, 25]. An interesting finding in the present study is the triple-$Q$ CO states. In these states, magnetic moments dominantly appear at charge-poor sites, forming the noncoplanar triple-$Q$ order, as schematically shown in Fig. 2. This is in sharp contrast to the collinear AF order in the CO state on a 2D square lattice [22]. The noncoplanar magnetic ordering is presumably due to the emergent frustration under CO; the charge-poor sites comprise a frustrated FCC lattice in the present cubic case, in contrast to the unfrustrated square lattice in the 2D case. It is interesting to note that a similar triple-$Q$ state and associated anomalous quantum Hall effect were discussed for the double-exchange model on a (distorted) FCC lattice [3, 26].

Let us closely discuss the electronic state in the triple-$Q$ magnetically-ordered phase (without CO) in Fig. 2.
face states emergent in the triple-

FIG. 4. (color online). (a)-(d) Intensity of the single-particle spectral functions $A_{sf}(k',\omega)$ at $E = 0.2$, 0.0, $-0.1$, and $E'$, respectively [see Fig. 3(d)]. We take the broadening factor $\delta = 0.03$. The thin lines show the constant energy contours at each $E$, and the hatched regions show the bulk states.

First, we show the band structure in the triple-$Q$ state in Fig. 3(a). Each band is doubly degenerate, and there are totally 16 bands. As shown in Fig. 3(a), 3D massless Dirac nodes appear at the $P$ point, in similar to Fig. 1(a). Following the arguments after Eq. (3), we confirmed the emergence of essentially the same Dirac electrons as in Eq. (5).

Next, we investigate the surface states peculiar to the triple-$Q$ order. We here consider the system with the $(110)$ surfaces, in which both top and bottom surfaces consist of A and C sublattice sites [27]; the geometry viewed from the $z$ direction is schematically shown in Fig. 3(b). Figures 3(c) and 3(d) show the band dispersions of the system with the $(110)$ surfaces [28]. The Dirac nodes at the $P$ point in the bulk system are projected onto $k' \equiv (k'_x/\sqrt{2}, k'_y) = (0, \pi/2)$, as shown in Figs. 3(c) and 3(d) [see Fig. 3(b) for the relation between $k$ and $k'$]. Between the bulk states, there appear four bands crossing the Fermi level. These are the gapless surface states emergent in the triple-$Q$ state with 3D Dirac electrons. The four bands meet at $(\pi/2, \pi/2)$ (we set this energy $E'$), whereas this point is not a Dirac node as the band dispersion in the $(\pi/2, \pi/2)-(0, \pi/2)$ direction is not linear but quadratic in $k'$, as shown in Fig. 3(d).

The resultant Fermi surfaces are shown by the thin lines in Fig. 4(b). They have closed forms, which converge to a single point at the Dirac nodes at the zone edges, $k' = (0, \pi/2)$ and $(\pi, \pi/2)$. The topology of the Fermi surfaces, however, changes drastically while shifting the Fermi level in a rigid band picture, as demonstrated in Fig. 4. To illustrate the contributions from surface states, we also show the intensity of single-particle spectral function at one of the two surfaces by the contours in Fig. 4. The spectral function is defined as $A_{sf}(k',\omega) = -\frac{1}{\pi} \text{Tr}_{sf}[\text{Im}(\omega + i\delta - \mathcal{H}(k'))^{-1}]$, where the trace $\text{Tr}_{sf}$ is taken only for the surface states at one of the surfaces and $\delta$ is a broadening factor. As shown in Fig. 4, this analysis clearly shows that the surface states do not have the ordinary closed Fermi surfaces but have the Fermi “arcs”, which disappear around the bulk Dirac cones at $(0, \pi/2)$ and $(\pi, \pi/2)$. We note that the surface states decrease rapidly from the edge to the bulk; the wave function at $E'$ is the most localized at the surfaces. On the other hand, the wave function at the Fermi level [at $(0, \pi/2)$] is extended throughout the system. Such situations are similar to the case in zigzag-edged graphene nanoribbons [29, 30]. The characteristic surface states in the triple-$Q$ ordered state are observable by the angle-resolved photoemission spectroscopy, as was recently done for Tungsten, in which Dirac-cone-like surface states also appear [31]. Especially, the spin polarization due to the surface magnetic moments will be detected.

To summarize, we have discovered that a noncoplanar triple-$Q$ order induces three-dimensional massless Dirac electrons on a cubic lattice. The Dirac state is doubly degenerate, resulting in the realization of Weyl electrons when the degeneracy is lifted in applied magnetic field. In addition, we have shown that the triple-$Q$ ordered state is the ground state at the mean-field level in a wide parameter region in the periodic Anderson model. We also demonstrated peculiar surface states with Fermi “arcs”.

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