Two-orbital model for CeB$_6$

Dheeraj Kumar Singh

Harish-Chandra Research Institute - Chhatnag Road, Jhunsi, Allahabad 211019, India and Homi Bhabha National Institute, Training School Complex - Anushakti Nagar, Mumbai 400085, India

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Abstract – We describe a two-orbital tight-binding model with bases belonging to the $\Gamma_8$ quartet. It captures several characteristics of the Fermiology unravelled by the recent angle-resolved photoemission spectroscopic (ARPES) measurements on cerium hexaboride CeB$_6$ samples cleaved along different high-symmetry crystallographic directions, which includes the ellipsoid-like Fermi surfaces (FSs) with major axes directed along $\Gamma$-X. We calculate various multipolar susceptibilities within the model and identify the susceptibility that shows the strongest divergence in the presence of standard onsite Coulomb interactions and discuss its possible implication and relevance with regard to the signature of strong ferromagnetic correlations evident in various phases as shown by the recent experiments.

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Introduction. – Strongly correlated $f$-electron systems exhibit a wide range of ordering phenomena including various magnetic orderings as well as superconductivity [1,2]. However, they are notorious for possessing complex ordered phases or so called “hidden order”, which are sometimes not easily accessible experimentally because of the ordering of multipoles of higher rank such as electric quadrupolar, magnetic octupole, etc. than the rank-one magnetic dipole [3,4]. This marked difference from the correlated $d$-electron system is a result of otherwise a strong spin-orbit coupling existent in these systems. Recent predictions of samarium hexaboride (SmB$_6$) to be a topological Kondo insulator has led to an intense interest and activities in these materials [5].

CeB$_6$ with a simple cubic crystal structure is one of the most extensively studied $f$-electron system both theoretically as well as experimentally. Apart from the pronounced Kondo lattice properties, it undergoes two different types of ordering transition as a function of temperature despite its simple crystal structure [6]. First, there is a transition to the antiferroquadrupolar (AFQ) phase with ordering wave vector $Q_3 = (\pi, \pi, \pi)$ at $T_Q \approx 3.2$ K, which has long remained hidden to the standard experimental probes such as neutron diffraction [7–13]. The nature of the primary order parameter was clarified to be of $\Gamma_5^+$-type ($O_{yz}, O_{zx}, O_{xy}$), and an antiferrooctupolar order parameter of $\Gamma_2^-$-type ($O_{xyz}$) is induced in an external field [10,11]. The multipolar order parameters are supported by the fourfold degenerate 4$f$ crystalline electric field (CEF) ground state $\Gamma_8$. Adopting a localized approach, a large body of experimental results have been explained. Finally, another transition to the AFM phase with double $Q_2$ commensurate structure with $Q_2 = (\pi/2, \pi/2, 0)$ takes place at $T_N \approx 2.3$ K [14].

Significant progress has been made recently through the experiments in understanding the nature of the above-mentioned phases of CeB$_6$. Magnetic spin resonance, for instance, has been observed in the AFQ phase [15,16] with its origin attributed to the ferromagnetic correlations [17,18] as in the Yb compounds, e.g., YbRh [17], YbIr$_2$Si$_2$ [19], and one Ce compound CeRuPO [20]. On the other hand, according to a recent neutron-scattering (NS) experiment, the AFM phase is rather a coexistence phase consisting of AFQ ordering as well [21]. In another INS measurements, low-energy ferromagnetic fluctuations have been reported to be more intense than the mode corresponding to the magnetic ordering wave vector $Q_2$ in the AFM phase, which stays though with reduced intensity even in the pure AFQ phase [22]. In addition, ferromagnetic spin correlations have been observed above $T_Q$ by magnetization measurements [23]. The overall picture emerging from these experiments and the hot spot observed near $\Gamma$ by ARPES imply the existence of strong ferromagnetic fluctuations in various phases of CeB$_6$. 

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So far most of the theoretical studies have focused on the localized aspects of $4f$ electron while neglecting the itinerant character when investigating multipole orderings [10,13,24]. However, this may appear surprising because the estimates of density of states (DOS) for CeB$_6$ at the Fermi level from low-temperature specific heat measurement as well as from the effective mass measurement from de Haas-van Alphen (dHvA) gives a significantly larger value when compared to the paramagnetic metal such as LaB$_6$ provided that the FSs are considered the same in both the compounds [25]. In the temperature regime $T > T_Q$, it exhibits a typical dense Kondo behavior dominated by Fermi liquid with a Kondo temperature of the order of $T_N$ and $T_Q$ [26]. Moreover, a low energy dispersionless collective mode at $Q_1$, has been observed in the INS experiments, which is well within the single-particle charge gap present in the coexistence phase [21]. The existence of such spin excitons has been reported in several superconductors [27] as well as heavy-fermion compounds [28] previously, and the explanation for the origin of such modes has been provided in terms of correlated particle-hole excitation, a characteristics of the itinerant systems.

Recent advancement based on a full 3D tomographic sampling of the electronic structure by the ARPES has unraveled the FSs in the high-symmetry planes of cubic CeB$_6$ [29,30]. FSs are found to be the cross sections of the ellipsoids, which exclude the $Γ$-point and are bisected by the (100)-plane at $k_z = \pi$. The largest semi-principal axis of the ellipsoid coincides with $Γ$-X. Based on the FS characteristics, it has been suggested that multipole order may arise due to the nesting as the shifting of one ellipsoid by the nesting vector ($π, π, π$) into the void formed in between other three can result in a significant overlap. Interestingly, the features of FS bear several similarities to those of LaB$_6$, which has also been suggested by earlier estimates based mainly on the dHvA experiments [25,31] as well as from several band-structure calculations [32–34].

Despite various experimental works on the FSs of CeB$_6$, no theoretical studies of ordering phenomena have been carried out within the models based on the realistic electronic structure, and therefore the nature of instability or fluctuations that will arise in that case is of strong current interest. To address this important issue, we propose to discuss a two-orbital tight-binding model with energy levels belonging to the $Γ_8$ quartet. The model reproduces the experimentally measured FSs well along the high-symmetry planes namely (100), (110), etc., which are part of the ellipsoid-like three-dimensional FSs with the squarish cross sections. With this realistic electronic structure, we examine the nature of instability or fluctuations in the Hubbard-like model with standard on-site Coulomb interaction terms considered usually in a multiorbital system such as iron-based superconductors. This is accomplished by studying the behavior of the susceptibilities corresponding to the various multipolar moments.

**Model Hamiltonian.** — A single-particle state in the presence of strong spin-orbit coupling is defined by using the total angular momentum $j = 1 + s$, which yields a low-lying sextet and a high-lying octet for $j = 5/2$ and $7/2$, respectively in the case of $f$-electron with $l = 3$. Therefore, with the number of electrons $n$ being 1, it is the low-lying sextet, which is relevant in the case of $Ce^{3+}$ ions. These ions are in the octahedral environment with corners being occupied by the six B ions. Therefore, the sextet is further split into a $Γ_8$ quartet which forms the ground state of CeB$_6$ and a high-lying $Γ_7$ doublets separated by $\sim$500 K. The $Γ_8$ quartet involves two Kramers doublets and each doublet can be treated as spin-$\frac{1}{2}$ system [35].

Using $Γ_8$ quartet, kinetic part of our starting Hamiltonian is

$$\mathcal{H}_0 = -\sum_{ij} \sum_{\mu,\nu,\sigma,\sigma'} t_{ij}^{\mu\sigma,\nu\sigma'} f_{i\mu\sigma} f_{j\nu\sigma'} + \text{H.c.},$$

where $t_{ij}^{\mu\sigma,\nu\sigma'}$ are the hopping elements from orbital $\mu$ with pseudospin $\sigma$ at site $i$ to orbital $\nu$ with pseudospin $\sigma'$ at site $j$. The operator $f_{i\mu\sigma}$ ($f_{i\mu\sigma}^\dagger$) creates (destroys) a $f$ electron in the $\mu$ orbital of site $i$ with pseudo spin $\sigma$. These are given explicitly in terms of the $z$-components of the total angular momentum $j = 5/2$ as follows:

$$f_{i1\uparrow} = \sqrt{\frac{5}{6}} c_{i\uparrow} + \sqrt{\frac{1}{6}} c_{i\downarrow}^\dagger,$$

$$f_{i1\downarrow} = \sqrt{\frac{5}{6}} c_{i\downarrow} + \sqrt{\frac{1}{6}} c_{i\uparrow}^\dagger,$$

$$f_{i2\uparrow} = c_{i\downarrow} - c_{i\uparrow}^\dagger,$$

$$f_{i2\downarrow} = c_{i\uparrow} + c_{i\downarrow}^\dagger.$$  

As can be seen in fig. 1, $Γ_8$ orbitals are similar in structure to the $d$-orbitals $d_{x^2−y^2}$ and $d_{3z^2−r^2}$.

![Fig. 1: (Colour online) $Γ_8$(1) and $Γ_8$(2) orbitals with a similar structure as $d$-orbitals $d_{x^2−y^2}$ and $d_{3z^2−r^2}$, respectively.](image-url)

The kinetic energy after the Fourier transform can be expressed in terms of $Γ$ matrices defined as $Γ^{0,1,2,3,4,5} = (\tilde{τ}_0\tilde{σ}_0, \tilde{τ}_0\tilde{σ}_0, \tilde{τ}_x\tilde{σ}_0, \tilde{τ}_y\tilde{σ}_0, \tilde{τ}_y\tilde{σ}_0, \tilde{τ}_y\tilde{σ}_0)$, where $σ$s and $τ$s are Pauli’s matrices corresponding to the spin and orbital degrees of freedom, respectively. So that

$$\sum_k \Psi_k^\dagger H_k \Psi_k = \sum_k \sum_{i=0,1,...,5} \Psi_k^\dagger d_i(k) Γ_i^\dagger \Psi_k.$$  

Here, $\Psi_k^\dagger = (f_{k1\uparrow}^\dagger, f_{k2\uparrow}^\dagger, f_{k1\downarrow}^\dagger, f_{k2\downarrow}^\dagger)$ is the electron field with $d_i(k)$'s

$$d_i(k) = -\mu + 8t\phi_0(k) + \frac{28}{3} t'\phi'_0(k) + \frac{128}{9} t''\phi''_0(k),$$

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The chemical potential $\mu$ is set to be $-16.4$. The calculated electron dispersions $\epsilon(k)$, which corresponds to the band filling $n \approx 0.55$. Figure 3 shows FSs cut along different high-symmetry planes. It has an ellipse-like structure with major axis aligned along $\Gamma$-$X$ for the $(100)$-plane while touching each other along the $\Gamma$-$M$ direction. On the other hand, the parallel plane at $(0, 0, \pi)$ consists of a single squarish pocket around that point. The six-fold rotation symmetry for the $(110)$-plane, two large ellipse-like FSs surfaces are present with the major axes along the $\Gamma$-$Y$ direction while small pockets exist along the $\Gamma$-$X$ direction. The six-fold rotation symmetry is reflected by the six pockets along $(111)$-plane. All of them are obtained from the FSs shown in the whole Brillouin zone as in fig. 4. It consists of an ellipsoid-like FSs with the largest semi-principal axes coinciding with $\Gamma$-$X$, however, with a squarish cross section. It is not unexpected particularly because of the flatness of the two bands near $\Gamma$ contributing mostly to the DOS at the Fermi level. Interestingly, a hot spot near $\Gamma$ has been observed also in the ARPES measurements, which points towards the possibility of strong ferromagnetic fluctuations [30]. Here, the chemical potential is chosen to be $-16.4$ to obtain a better agreement with the ARPES FSs, which corresponds to the band filling $n \approx 0.55$.

In the absence of the second and third nearest-neighbor hopping, the kinetic part of the Hamiltonian reduces to that of manganites [36] with the only difference of a constant multiplication factor. In the following, the unit of energy is set to be $t$. The calculated electron dispersions for $t' = -0.38$ and $t'' = 0.18$, which consists of doubly degenerate eigenvalues, are shown in fig. 2(a) along the high-symmetry directions. A large electron pocket near $X$ and the extrema exhibited by two bands near $\Gamma$ just below the Fermi level are broadly in agreement with $4f$ dominated part in the band-structure calculations. The density of states (DOS) shows two peaks with the larger one being in the vicinity of the Fermi level (fig. 2(b)).

$$
\begin{align*}
\epsilon^1(k) &= 4t\phi_1(k) - \frac{2}{3}t'\phi^*_1(k), \\
\epsilon^2(k) &= -4\sqrt{3}\phi_2(k) + \frac{2}{\sqrt{3}}t'\phi^*_2(k), \\
\epsilon^3(k) &= \frac{16}{\sqrt{3}}t'\phi^*_3(k) + \frac{128}{9\sqrt{3}}t''\phi^*_5(k), \\
\epsilon^4(k) &= \frac{16}{\sqrt{3}}t'\phi^*_4(k) + \frac{128}{9\sqrt{3}}t''\phi^*_5(k). 
\end{align*}
$$

In the absence of the second and third nearest-neighbor hopping, the kinetic part of the Hamiltonian reduces to that of manganites [36] with the only difference of a constant multiplication factor. In the following, the unit of energy is set to be $t$. The calculated electron dispersions for $t' = -0.38$ and $t'' = 0.18$, which consists of doubly degenerate eigenvalues, are shown in fig. 2(a) along the high-symmetry directions. A large electron pocket near $X$ and the extrema exhibited by two bands near $\Gamma$ just below the Fermi level are broadly in agreement with $4f$ dominated part in the band-structure calculations. The density of states (DOS) shows two peaks with the larger one being in the vicinity of the Fermi level (fig. 2(b)).

\begin{align*}
\phi_0 &= \cos k_x + \cos k_y + \cos k_z, \\
\phi'_0 &= \cos k_y \cos k_x + \cos k_z \cos k_y + \cos k_x \cos k_y, \\
\phi_1 &= \cos k_x + \cos k_y - 2 \cos k_z, \\
\phi'_1 &= \cos k_y \cos k_x + \cos k_z \cos k_x - 2 \cos k_x \cos k_y, \\
\phi_2 &= \cos k_x - \cos k_y, \\
\phi'_2 &= \cos k_y \cos k_x - \cos k_z \cos k_x + 2 \cos k_x \cos k_y, \\
\phi_3 &= \sin k_y \sin k_z, \\
\phi'_3 &= \sin k_z \sin k_y, \\
\phi_4 &= \sin k_x \sin k_y, \\
\phi'_4 &= \sin k_y \sin k_x, \\
\phi_5 &= \cos k_x \cos k_y \cos k_z, \\
\phi'_5 &= \cos k_z \sin k_y \sin k_z, \\
\phi_6 &= \sin k_x \cos k_y \sin k_z, \\
\phi'_6 &= \sin k_y \sin k_x \cos k_x. 
\end{align*}

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the chemical potential

Fig. 4: (Colour online) Fermi surfaces in the Brillouin zone for

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Apart from the recent advancement in the ARPES measurements on this material, several new features have emerged in the NS measurements, which may provide crucial information regarding the scattering by magnetic multipoles or odd-rank multipoles. The component of the scattering operator \( Q \), in general, can be defined as [37]

\[
Q_\alpha = a(k') \left( J_{\alpha}^1 + \sum_{\beta} b_{\alpha\beta}(k') J_{\beta}^3 \right),
\]

where \( J_{\alpha}^1 \) and \( J_{\alpha}^3 \) are the dipolar and octupolar operators, respectively. \( a(k') \) is a decreasing function of momentum transfer \( k' = |k'| = |k_1 - k_2| \) such that \( a(k') < a(0) \). Note that the Landé \( g \)-factor is absorbed in \( a(k') \). Further details of matrix elements of the scattering operators can be found in earlier works. Here, it is also important to note that AFQ order can also be detected using NS experiments though indirectly because of the induced magnetic order or octupole order in this material.

In the following, we describe the multipolar susceptibilities directly related to the NS measurements with the model presented in this work. Our focus is the unordered state. Earlier, Lindhard function has been calculated in the unordered state with the electronic structure fitted to the ARPES FSs, which shows three main peaks near \( (\pi, 0, 0) \), \( (\pi/2, \pi/2, 0) \) and \( Q_1 \) [29]. Since the model is a one-band model, it is not possible to define multipolar susceptibilities, and therefore it remains unclear as to what type of instabilities or strong fluctuations corresponding to the above-mentioned wave vectors exist.

**Multipolar susceptibilities.**—Sixteen multipolar moments can be defined for the \( \Gamma_8 \) state including one charge, three dipoles, five quadrupoles and seven octupoles, which are rank-0, rank-1, rank-2 and rank-3 tensors, respectively. The dipole belongs to the \( \Gamma_4 \) irreducible representation, where the \(-\) sign denotes the breaking of time-reversal symmetry. Its components are given by the outer product of Pauli’s matrices \( \hat{\tau}_0 \hat{\sigma}_1 \). The quadrupole moments belonging to \( \Gamma_5^+ \) are \( \hat{\tau}_z \hat{\sigma}_0 \) and \( \hat{\tau}_x \hat{\sigma}_0 \) while those belonging to \( \Gamma_5^- \) irreducible representations are expressed as \( \hat{\tau}_y \hat{\sigma}_0 \). The octupole moment with \( \Gamma_5^+ \) representation is \( \hat{\tau}_z \hat{\sigma}_0 \), whereas the \( z \)-components of those belonging to \( \Gamma_5^- \) and \( \Gamma_5^z \) are \( 2\hat{\tau}_z \hat{\sigma}_z \) and \( 2\hat{\tau}_z \hat{\sigma}_z \), respectively.

In order to examine the multipolar ordering instabilities, we calculate susceptibilities while considering only the \( z \)-component whenever components along the three coordinate axes are present, as that will be sufficient because of the cubic symmetry. Multipolar susceptibilities are defined as [38]

\[
\chi^{\mu\nu;rs}(q, i\omega_n) = \frac{1}{\beta} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau [O_{q}^{\mu\nu}(\tau)O_{-q}^{rs}(0)] \rangle, 
\]

where

\[
O_{q}^{\mu\nu} = \sum_{k} \sum_{\sigma'} \sum_{\mu'} f_{\mu\sigma'}^{\mu'}(k + q) f_{\mu'\sigma'}^{\mu'}(k), \quad (8)
\]

They can be expressed in terms of

\[
\chi^{\sigma\sigma;\sigma\sigma}(q, i\omega_n) = \frac{1}{\beta} \int_0^\beta d\tau \sum_k \sum_{\tau'} \langle T_\tau f_{kq\mu\sigma}^{\mu\sigma}(\tau) f_{k'q'\mu'\sigma'}^{\mu'\sigma'}(0) \langle k' \rangle \rangle, \quad (9)
\]

which forms a 16×16 matrix. Thus, the dipole or spin susceptibility is given by

\[
\chi^{0z;0z}(q, i\omega_n) = \sum_{\sigma'\mu'} \chi^{\sigma\sigma;\sigma'\sigma'}(q, i\omega_n) \langle k \rangle, \quad (10)
\]

where \( \sigma \) and \( \mu \) in front of \( \chi \) take \(+1\) or \(-1\) values corresponding to the two spin or orbital degrees of freedom. Various quadrupolar and octupolar susceptibilities are given as

\[
\chi^{x0;0z}(q, i\omega_n) = \sum_{\sigma\mu'} \chi^{\sigma\sigma;\sigma'\mu'}(q, i\omega_n), \quad (11)
\]

and

\[
\chi^{y0;0x}(q, i\omega_n) = -i^2 \sum_{\sigma'\mu'} \chi^{\sigma\sigma;\sigma'\mu'}(q, i\omega_n), \quad (12)
\]

respectively.

Figure 5 shows different static multipolar susceptibilities with well-defined peaks for some \( Q \)'s while broad hump-like structure for the other. Particularly, the spin susceptibility \( \chi^{0z;0z} \) is, among all, sharply peaked,
however, at $\approx Q_3 = (0, 0, 0)$. The quadrupolar susceptibility $\chi^{yz,yz}_{zz,zz}$ is peaked near $\approx Q_3$ while $\chi^{xyz,xyz}$ has a broad hump-like structure near $(\pi, 0, 0)$ and a peak near $Q_1$. We further note that $\chi^{xyz,xyz} = \chi^{yz,yz}$ and $\chi^{xyz,xyz}$ as shown in fig. 5(b).

It is worthwhile to note that the peak positions obtained here are largely in agreement with those obtained with the one-band model [29]. Importantly, it can be easily seen which multipolar susceptibilities are responsible for the peak structures at the various wave vectors. Moreover, we also find strong ferromagnetic instability otherwise absent in the one-band model, which may be helpful in understanding the ferromagnetic correlations and fluctuations in various phases including the paramagnetic one, as observed in several experiments.

**Multipolar susceptibilities in the presence of interaction.** – In order to investigate the role of electron-electron correlation, we consider the standard onsite Coulomb interaction terms given as [39]

$$H_{\text{int}} = U \sum_{i,\mu} n_{i\mu} n_{i\mu} + (U' - \frac{J}{2}) \sum_{i,\mu < \nu} n_{i\mu} n_{i\nu} - 2J \sum_{i,\mu < \nu} S_{i\mu} \cdot S_{i\nu} + J \sum_{i,\mu < \nu, \sigma} f_{i\mu\sigma} \dagger f_{i\mu\sigma} f_{i\nu\sigma} \dagger f_{i\nu\sigma}. \quad (13)$$

Figure 6 shows the multipolar static susceptibilities at the RPA-level. As expected, the RPA spin susceptibility

\[ \chi_{R}(q, i\omega) = (\hat{1} - \hat{U} \chi(q, i\omega))^{-1} \chi(q, i\omega). \quad (14) \]

Here, $\hat{1}$ is a 16$\times$16 identity matrix, whereas the interaction matrix $U'_{\mu_1,\nu_1;\mu_2,\nu_2}$ is given by [40]

\[
\begin{align*}
-U & \quad (\mu_1 = \mu_2 = \mu_3 = \mu_4, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
-U' & \quad (\mu_1 = \mu_2 \neq \mu_3 = \mu_4, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
-J & \quad (\mu_1 = \mu_4 \neq \mu_2 = \mu_3, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
-J' & \quad (\mu_1 = \mu_3 \neq \mu_2 = \mu_4, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
-(U - J'') & \quad (\mu_1 = \mu_2 \neq \mu_3 = \mu_4, \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4), \\
(U - J') & \quad (\mu_1 = \mu_4 \neq \mu_2 = \mu_3, \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4), \\
U & \quad (\mu_1 = \mu_2 = \mu_3 = \mu_4, \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4), \\
U' & \quad (\mu_1 = \mu_4 \neq \mu_2 = \mu_3, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
J & \quad (\mu_1 = \mu_2 \neq \mu_3 = \mu_4, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
J' & \quad (\mu_1 = \mu_3 \neq \mu_2 = \mu_4, \sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4), \\
0 & \quad \text{(otherwise)}. \\
\end{align*}
\]

in a manner similar to the various correlated multiorbital systems. The first term represents the intraorbital Coulomb interaction for each orbital. The second and third terms represent the density-density interaction and Hund’s coupling between the two orbitals, respectively. The fourth term represents the pair-hopping energy whereas the condition $U'' = U - 2J$ is essential for the rotational invariance.

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Interestingly, it diverges near $Q_3$ instead of at the AFM ordering wave vector $Q_2$, which is not surprising because there exists a large DOS near $\Gamma$ that leads also to the peak near $Q_3$ in bare spin susceptibility. Thus, AFQ instability corresponding to the $\Gamma_8^2$ representation is absent in the model despite the bare quadrupole susceptibility being peaked near $Q_1$. However, we believe that the strong low-energy ferromagnetic fluctuations in the paramagnetic phase may have important implications for the persistent ferromagnetic correlations in various ordered phases as observed by various experiments [16,22].

Conclusions and discussions. – In conclusion, we have described a tight-binding model with the bases as $\Gamma_5$, which captures the salient features of the Fermi surfaces along the high-symmetry planes as observed in the ARPES measurements. A large density of state is obtained near the Fermi level due to the flatness of the bands close to $\Gamma$, which bears a remarkable similarity to the hot spot observed in another ARPES experiments. Multipolar susceptibilities calculated with the standard onsite Coulomb interactions as in other multiorbital systems show that it is the spin susceptibility that exhibits the strongest diverging behavior. Moreover, it does so in the low-momentum region implying an underlying ferromagnetic instability.

It is clear that the nature of the instability obtained with the realistic electronic structure is different from the actual order in CeBa, which agrees with the ferromagnetic correlations observed in the paramagnetic phase. However, it is important to note that some of the recent experiments have provided the evidence of strong ferromagnetic correlations in the ordered phases. For instance, there exists magnetic spin resonance in the AFQ phase, which has been attributed to the FM correlations. Further, the most intense spin-wave excitation modes have been observed at zero-momentum instead of the AFM ordering wave vector by the INS measurements in the coexistence phase, which continues to be present even in the AFQ phase. A similar INS measurement in the paramagnetic phase is highly desirable to probe the existence of ferromagnetic correlations in the paramagnetic phase. It is to be noted that an indirect indication in the form of hot spot observed by ARPES near $\Gamma$ is also available. In order to understand the above-mentioned features, we believe that the strong low-energy ferromagnetic fluctuations obtained within the two-orbital model with the realistic electronic structure may be an important step. To explain AFQ and other multipole order, it would perhaps be necessary to include the local-exchange terms involving quadrupolar and multipolar moments, which should be the subject matter of future investigation.

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