Spin Exciton Formation inside the Hidden Order Phase of CeB_6

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The heavy fermion metal CeB_6 exhibits a hidden order of the antiferroquadrupolar (AFQ) type below $T_Q = 3.2$ K and a subsequent antiferromagnetic (AFM) order at $T_N = 2.3$ K. It was interpreted as an ordering of the quadrupole and dipole moments of a Γ_8 quartet of localized Ce $4f^1$ electrons. This established picture has been profoundly shaken by recent inelastic neutron scattering (G. Friemel *et al.*, arXiv:1111.4151) that found the evolution of a feedback spin exciton resonance within the hidden order phase at the AFQ wave vector which is stabilized by the AFM order. We develop an alternative theory based on a fourfold degenerate Anderson lattice model, including both order parameters as particle-hole condensates of itinerant heavy quasiparticles. This explains in a natural way the appearance of the spin exciton resonance and the momentum dependence of its spectral weight, in particular, around the AFQ vector and its rapid disappearance in the disordered phase. Analogies to the feedback effect in unconventional heavy fermion superconductors are pointed out.

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In strongly correlated f-electron metals, the investigation of the hidden order (HO) of the unconventional nonmagnetic type is a topic of central importance [1]. The most prominent and most investigated heavy fermion compounds that exhibit HO at low temperatures are URu_2Si_2 and CeB_6 which have tetragonal (D_{4h}) or cubic (O_h) structure, respectively. Two issues arise in the context of hidden order. First, which symmetry is broken in the HO phase and to which irreducible representation does the order parameter belong? Second, should the ordering be described as the appearance of spontaneous long-range correlation between local f-electron degrees of freedoms, i.e., f-electron multipoles, or should HO rather be described as the condensation of itinerant heavy particle-hole pairs with a nontrivial orbital structure? These opposite perspectives have prevented a clear identification of the HO in URu_2Si_2 until the present.

On the other hand, since the work of Ohkawa [2], the HO in CeB_6 which appears at $T_Q = 3.2$ K has always been taken for granted as a paradigm of the localized HO picture. In subsequent work along this line [3,4], it was clarified that the primary HO parameter is of the two-sublattice antiferroquadrupolar (AFQ) Γ_5^+ type (O_{yz}, O_{zx}, O_{xy}), with a wave vector $\mathbf{Q}' = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in reduced lattice units (R point) which is nearly degenerate, with an antiferrooctupolar (AFO) Γ_2^- (T_{xyz}) order parameter which is strongly induced in an external field. Here, $\pm$ denotes the parity with respect to time reversal. The hidden multipolar order parameters are supported by the fourfold degenerate $4f$ crystalline electric field (CEF) ground state Γ_8. This localized scenario explains a large body of experimental results, including the field-dependent increase and anisotropy of the critical temperature and the field-induced Bragg peaks [5] at $\mathbf{Q}'$ and NMR line shifts [4], although there is no macroscopic symmetry breaking observed [6]. A further important support for this picture comes from the predicted rapid field-induced increase of the secondary octupole order parameter [3] which was directly confirmed by resonant x-ray scattering experiments [7]. At temperatures below $T_N = 2.3$ K, CeB_6 finally develops antiferromagnetism (AFM) with $\mathbf{Q} = (\frac{1}{4}, \frac{1}{4}, 0)$ (Σ or S point) that coexists with AFQ order. Important information on HO may also be gained from the magnetic excitation spectrum. For finite fields that stabilize the AFQ/AFO HO, it was investigated within generalized Holstein-Primakoff and random phase approximation (RPA) approaches [8,9]. Both lead to multipolar excitation bands in the range of 1–2.5 meV, and, for finite applied fields [10], their salient features agree with experimental results from inelastic neutron scattering (INS). In the numerous theoretical investigations of HO in CeB_6, the localized $4f$ approach was chosen and itinerant $4f$ character was completely neglected. This seems surprising because CeB_6 is a prominent example of a heavy fermion metal with one of the heaviest masses reported ($m^*/m \geq 17$) [11] and because the Ce dilute La substitutes [12] are the standard case of Kondo resonance-dominated local Fermi liquids with all the typical Kondo anomalies identified there. In fact, the estimated Kondo temperature of the concentrated CeB_6 from quasielastic neutron scattering [13] is $T^* \simeq 4.5$ K, which is of the same order as T_Q and T_N. Therefore, one question is whether the HO physics of CeB_6 can be completely explained within the conventional localized $4f$ approach.

Recent zero-field high-resolution INS experiments by Friemel *et al.* [14] have indeed seriously questioned the standard picture and found intriguing new evidence that the dynamical magnetic response in the HO phase cannot be understood in the localized approach and, as in URu_2Si_2, requires taking into account the itinerant quasiparticle nature of f electrons. It was found that the low-temperature magnetic response within the HO phase is determined by a pronounced *feedback effect*, i.e., a modification of magnetic spectral properties due to the appearance of order parameters: (i) Below T_N, a spin gap opens for low energies and spectral weight from the quasielastic region [15] is shifted to higher energies, forming a pronounced resonance at $\mathbf{Q}'$ with peak position $\omega_r \simeq 0.5$ meV. (ii) Using the single-particle charge gap $2\Delta \simeq 1.2$ meV in the HO phase from point-charge spectroscopy [16], $\omega_r/2\Delta = 0.42 < 1$ is fulfilled, showing that the resonance is indeed split off from the continuum. (iii) The resonance appears mainly at the AFQ $\mathbf{Q}'$ but not at the AFM $\mathbf{Q}$ vector and shows no dispersion. Its intensity decreases rapidly when approaching T_N from below in an order-parameter-like fashion. These characteristics of the magnetic spectrum in CeB_6 do not suggest a spin wave origin but rather are reminiscent of spin exciton resonances observed before in Fe pnictides [17] and heavy fermion superconductors [18,19], as well as Kondo insulators [20,21]. The results of Ref. [14] are the first clear-cut example of the feedback spin exciton appearing within the AFQ HO phase. This proves that the localized $4f$ scenario for CeB_6 is not adequate to explain its intriguing low-energy spin dynamics and its momentum dependence.

In this Letter, we therefore propose and explore an alternative route of theoretical modeling. We start from the central idea that the AFQ and AFM order parameters are to be described as particle-hole condensates in the itinerant heavy quasiparticle picture. The latter is obtained from a microscopic fourfold (Γ_8-type) degenerate Anderson lattice model. It includes both twofold pseudospin ($\sigma = \uparrow, \downarrow$) and twofold pseudo-orbital ($\tau = \pm$) degeneracies of the hybridizing conduction (c) and $4f$ electron (f) in the Γ_8 CEF ground state according to

$$\mathcal{H} = \sum_{\mathbf{k},m}[\epsilon^c_{\mathbf{k}} c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \epsilon^f_{\mathbf{k}} f^\dagger_{\mathbf{k}m} f_{\mathbf{k}m} + V_{\mathbf{k}}(c^\dagger_{\mathbf{k},m} f_{\mathbf{k}m} + \mathrm{H.c.})] + \sum_{i,m,n} U_{ff} f^\dagger_{im} f_{in} f^\dagger_{in} f_{im}, \quad (1)$$

where $m = (\tau, \sigma)$ represents the fourfold Γ_8 degeneracy. Here, $c^\dagger_{\mathbf{k}m}$ creates a conduction electron in the channel with corresponding Γ_8 symmetry and wave vector $\mathbf{k}$. Furthermore, $\epsilon^c_{\mathbf{k}}$ and $\epsilon^f_{\mathbf{k}} = \epsilon^f$ are effective tight binding dispersions of the conduction band and the atomic f level position, respectively. For the former, we restrict to the next-neighbor hopping (t), i.e., $\epsilon^c_{\mathbf{k}} = 2t\sum_n \cos k_n$ ($n = x, y, z$), which leads naturally to the AFQ ordering vector $\mathbf{Q}'$. Furthermore, $f^\dagger_{\mathbf{k}m}$ creates the f electron with momentum $\mathbf{k}$, and U_{ff} is its on-site Coulomb repulsion. Finally, $V_{\mathbf{k}}$ is the hybridization energy between the lowest $4f$ doublet and conduction bands which contains in principle the effects of spin orbit and the CEF but is taken as constant $V_{\mathbf{k}} = V$ here.

In the limit $U_{ff} \to \infty$, double occupation of the f states is excluded; this is achieved by using the auxiliary boson b_i at each site i, with the constraint $b^\dagger_i b_i + \sum_m f^\dagger_{im} f_{im} = 1$. In the mean field (MF) approximation ($r = \langle b_i \rangle = \langle b^\dagger_i \rangle$), diagonalization leads to hybridized quasiparticle bands [12]. They are determined by the renormalized f level $\tilde{\epsilon}^f_{\mathbf{k}} = \epsilon^f_{\mathbf{k}} + \lambda$ and the effective (reduced) hybridization $\tilde{V}_{\mathbf{k}} = rV_{\mathbf{k}}$. Minimizing the MF ground-state energy leads to self-consistent equations for r and λ.

The AFQ and AFM order parameters with wave vectors $\mathbf{Q}$ and $\mathbf{Q}'$ respectively contribute extra MF terms:

$$\mathcal{H}_{\mathrm{AFQ}} = \sum_{\mathbf{k}\sigma} \Delta_{\mathbf{Q}'}(f^\dagger_{\mathbf{k},+\sigma} f_{\mathbf{k}+\mathbf{Q}'-\sigma} + f^\dagger_{\mathbf{k},-\sigma} f_{\mathbf{k}+\mathbf{Q}',+\sigma}),$$
$$\mathcal{H}_{\mathrm{AFM}} = \sum_{\mathbf{k}\tau} \Delta_{\mathbf{Q}}(f^\dagger_{\mathbf{k}\tau\uparrow} f_{\mathbf{k}+\mathbf{Q}\tau\downarrow} + f^\dagger_{\mathbf{k}\tau\downarrow} f_{\mathbf{k}+\mathbf{Q}\tau\uparrow}). \quad (2)$$

Our emphasis in this work is on the feedback effect, i.e., the effect of the gap opening within the HO phase on the magnetic response. Therefore, we do not attempt a microscopic calculation to derive these order parameters and their temperature dependence. We include them as symmetry breaking molecular field terms in the Hamiltonian and take a generic empirical temperature dependence. The MF Hamiltonian $\mathcal{H}_{\mathrm{MF}}$ obtained from Eq. (1) is diagonalized by the unitary transformation

$$f_{\mathbf{k}m} = u_{+,\mathbf{k}} a_{+,\mathbf{k}m} + u_{-,\mathbf{k}} a_{-,\mathbf{k}m},$$
$$c_{\mathbf{k}m} = u_{-,\mathbf{k}} a_{+,\mathbf{k}m} - u_{+,\mathbf{k}} a_{-,\mathbf{k}m}, \quad (3)$$

where $2u^2_{\pm,\mathbf{k}} = 1 \pm (\epsilon^c_{\mathbf{k}} - \tilde{\epsilon}^f_{\mathbf{k}})/\sqrt{(\epsilon^c_{\mathbf{k}} - \tilde{\epsilon}^f_{\mathbf{k}})^2 + 4\tilde{V}^2_{\mathbf{k}}}$, leading to $\mathcal{H}_{\mathrm{MF}} = \sum_{i,\mathbf{k},m} E^\alpha_{\mathbf{k}} a^\dagger_{\alpha,\mathbf{k}m} a_{\alpha,\mathbf{k}m} + \lambda(r^2 - 1)$, where $E^\pm_{\mathbf{k}} = \frac{1}{2}[\epsilon^c_{\mathbf{k}} + \tilde{\epsilon}^f_{\mathbf{k}} \pm \sqrt{(\epsilon^c_{\mathbf{k}} - \tilde{\epsilon}^f_{\mathbf{k}})^2 + 4\tilde{V}^2_{\mathbf{k}}}]$ is the pair (($\alpha = \pm$) of hybridized quasiparticle ($a_{\alpha\mathbf{k}m}$) bands and each fourfold ($m = 1$–4) is degenerate. Here, $\tilde{V}^2_{\mathbf{k}} = V^2_{\mathbf{k}}(1 - n_f)$ denotes the effective hybridization obtained by projecting out double occupancies. Because of $1 - n_f \ll 1$, $\tilde{V}_{\mathbf{k}}$ is strongly reduced with respect to the single particle $V_{\mathbf{k}}$ which leads to the large quasiparticle mass. Introducing new Nambu operators as $\psi^\dagger_{\mathbf{k}} = (C^\dagger_{\mathbf{k}}, C^\dagger_{\mathbf{k}+\mathbf{Q}'}, C^\dagger_{\mathbf{k}+\mathbf{Q}})$, where $C^\dagger_{\mathbf{k}} = (b^\dagger_{+,\mathbf{k}}, b^\dagger_{-,\mathbf{k}})$ and $b^\dagger_{\alpha,\mathbf{k}} = (a^\dagger_{\alpha,\mathbf{k}+\uparrow}, a^\dagger_{\alpha,\mathbf{k}+\downarrow}, a^\dagger_{\alpha,\mathbf{k}-\uparrow}, a^\dagger_{\alpha,\mathbf{k}-\downarrow})$, we can write the total Hamiltonian $\mathcal{H}_{\mathrm{tot}} = \mathcal{H}_{\mathrm{MF}} + \mathcal{H}_{\mathrm{AFQ}} + \mathcal{H}_{\mathrm{AFM}}$ as

$$\mathcal{H}_{\mathrm{tot}} = \sum_{\mathbf{k}} \hat{\psi}^\dagger_{\mathbf{k}} \hat{\beta}_{\mathbf{k}} \hat{\psi}_{\mathbf{k}};$$
$$\hat{\beta}_{\mathbf{k}} = \begin{bmatrix} \hat{E}_{\mathbf{k}} & \hat{\Delta}_{\mathbf{Q}'} & \hat{\Delta}_{\mathbf{Q}} \\ \hat{\Delta}_{\mathbf{Q}'} & \hat{E}_{\mathbf{k}+\mathbf{Q}'} & 0 \\ \hat{\Delta}_{\mathbf{Q}} & 0 & \hat{E}_{\mathbf{k}+\mathbf{Q}} \end{bmatrix}.$$

Here, $\hat{E}_{\mathbf{k}} = \hat{\mathcal{E}}_{\mathbf{k}} \otimes \tau_0 \otimes \sigma_0$, $\hat{\Delta}_{\mathbf{Q}'} = \Delta_{\mathbf{Q}'}(\hat{\rho}_{\mathbf{k},\mathbf{Q}'} \otimes \hat{\tau}_0 \otimes \hat{\sigma}_x)$, and $\hat{\Delta}_{\mathbf{Q}} = \Delta_{\mathbf{Q}}(\hat{\rho}_{\mathbf{k},\mathbf{Q}} \otimes \hat{\tau}_x \otimes \hat{\sigma}_0)$, where $\hat{\mathcal{E}}_{\mathbf{k}}$ and $\hat{\rho}_{\mathbf{k},\mathbf{Q}'}$ are 2×2 matrices in $\alpha = \pm$ space with matrix elements

$\hat{\mathcal{E}}^{\alpha\beta}_{\mathbf{k}} = \delta_{\alpha\beta} E^{\alpha}_{\mathbf{k}}$ and $\hat{\rho}^{\alpha\beta}_{\mathbf{k},\mathbf{k}'} = u_{\alpha\mathbf{k}} u_{\beta,\mathbf{k}+\mathbf{k}'}$. σ_l and τ_l are the Pauli matrices acting in pseudospin and pseudo-orbital space, respectively.

Defining the Matsubara Green's function matrix as $\hat{G}_{\mathbf{k}}(\tau) = -\langle T \hat{\psi}_{\mathbf{k}}(\tau) \hat{\psi}^{\dagger}_{\mathbf{k}}(0)\rangle$ and solving the standard equations of motion, one can find $\hat{G}_{\mathbf{k}}(\omega_n) = (i\omega_n - \hat{\beta}_{\mathbf{k}})^{-1}$, which can be written as

$$\hat{G}_{\mathbf{k}}(\omega_n) = \begin{bmatrix} \hat{G}^0_{\mathbf{k}} & \hat{G}^0_{\mathbf{k},\mathbf{k}+\mathbf{Q}'} & \hat{G}^0_{\mathbf{k},\mathbf{k}+\mathbf{Q}} \\ \hat{G}^0_{\mathbf{k}+\mathbf{Q}',\mathbf{k}} & \hat{G}^0_{\mathbf{k}+\mathbf{Q}'} & \hat{G}^0_{\mathbf{k}+\mathbf{Q}',\mathbf{k}+\mathbf{Q}} \\ \hat{G}^0_{\mathbf{k}+\mathbf{Q}\mathbf{k}} & \hat{G}^0_{\mathbf{k}+\mathbf{Q},\mathbf{k}+\mathbf{Q}'} & \hat{G}^0_{\mathbf{k}+\mathbf{Q}} \end{bmatrix}. \tag{4}$$

Here, $\hat{G}^0_{\mathbf{k}}$ is an 8×8 Green's function matrix in (α, m) space. For the magnetic excitation spectrum, we need the dipolar susceptibility matrix given by $\chi^{ll'}_{\mathbf{q}}(t) = -\theta(t) \times \langle T j^l_{\mathbf{q}}(t) j^{l'}_{-\mathbf{q}}(0)\rangle$, where $j^l_{\mathbf{q}} = \sum_{\mathbf{k}mm'} f^{\dagger}_{\mathbf{k}+\mathbf{q}m} \hat{M}^l_{mm'} f_{\mathbf{k}m'}$ are the physical magnetic dipole operators $(l, l' = x, y, z)$. In cubic symmetry, it is sufficient to calculate $\chi^{zz}_{\mathbf{q}}(\omega)$, corresponding to [9] $\hat{M}^z = \frac{7}{6}\hat{\tau}_0 \otimes \hat{\sigma}_z$; defining $s = (\alpha, \mathbf{k} + \mathbf{q}, m_1)$ and $s' = (\alpha', \mathbf{k}, m_2)$, one finds

$$\chi_0(\mathbf{q}, \omega) = \chi^{zz}_{\mathbf{q}}(\omega) \propto \sum_{\alpha\alpha'\mathbf{k}m_1m_2} (\hat{\rho}^{\alpha'\alpha}_{\mathbf{k},\mathbf{q}})^2 \times \int d\omega' \hat{G}^0_{ss}(\nu + \omega') \hat{G}^0_{s's'}(\omega')|_{i\nu \to \omega + i0^+}. \tag{5}$$

Here, the $\hat{\rho}^{\alpha'\alpha}_{\mathbf{k},\mathbf{q}}$ are the matrix elements of reconstructed quasiparticle states in the AFQ/AFM state. They play a similar role as the "coherence factors" in the spin exciton formation in unconventional superconductors. The dynamic magnetic susceptibility in RPA has the form

$$\chi_{\mathrm{RPA}}(\mathbf{q}, \omega) = [1 - J_{\mathbf{q}} \chi^{zz}_{\mathbf{q}}(\omega)]^{-1} \chi^{zz}_{\mathbf{q}}(\omega), \tag{6}$$

where $J_{\mathbf{q}}$ is the heavy quasiparticle interaction taken diagonal in (α, m) band indices. In principle, it is determined by processes beyond the slave boson MF approximation [22]. However, as in other spin exciton theories [21,23], we adopt here an empirical form of Lorentzian type that is peaked at the AFQ ordering vector where the resonance appears.

We will now discuss the characteristics of the magnetic excitation spectrum obtained from $\chi''_{\mathrm{RPA}}(\mathbf{q}, \omega)$ and show that it explains all the essential experimental features observed in $\mathrm{CeB_6}$. In accordance with the heavy quasiparticle mass in this compound, the chemical potential is chosen close to the top of the lower quasiparticle band [Fig. 1(a) inset: $\mu = -0.06t$] where dispersion is flat, leading to a realistic mass enhancement $m^*/m \simeq 20$. All other model parameters are defined in Fig. 1.

First, the spectrum $\chi''_0(\mathbf{q}, \omega)$ of *noninteracting* quasiparticles is shown in Fig. 1(a) with constant $\mathbf{q}$ scans for the paramagnetic (PM), AFQ, and coexistent AFQ/AFM phases, respectively. In the PM state, the spectrum exhibits the cf hybridization gap at the R point. When the AFQ and AFM orders appear, their corresponding gaps $\Delta_{\mathbf{Q}'}$ and $\Delta_{\mathbf{Q}}$ push the magnetic response to higher energies. The associated real part in Fig. 1(b) then shows a much-enhanced response at these energies. As a consequence, the magnetic spectrum for the *interacting* quasiparticles may develop a resonance when the real part of the denominator in Eq. (6) is driven to zero, equivalent to a pole in $\chi_{\mathrm{RPA}}(\mathbf{Q}', \omega)$. Because of the 3D electronic structure, $\chi'_0(\mathbf{Q}', \omega)$ will not be singular and the resonance will only appear for $J(\mathbf{Q}')$ larger than a threshold value. The imaginary part is generally nonzero but small, leading to a large resonant response at the pole position. The resonance appears in the HO phase when $J_{\mathbf{Q}'}/t$ lies in a reasonable range such that the pole exists only when the real part is enhanced by the gap formation. Then, the resonance condition $1 = J_{\mathbf{Q}'} \chi_0(\mathbf{Q}', \omega_r)$ is fulfilled only in the AFQ ordered regime. The magnetic spectrum of interacting quasiparticles is shown in Fig. 1(c). It shows indeed a peak appearing in the AFQ phase and a sharp resonant peak at $\omega_r/2\Delta_c = 0.64$ at low temperature when both gaps are present. Here, $\Delta_c = 0.056t$ is the charge gap given in the inset of

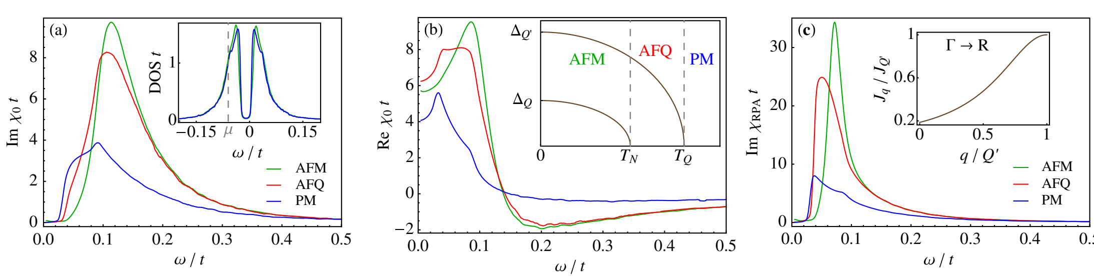

FIG. 1 (color online). Noninteracting susceptibility at the R point $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$: (a) is the imaginary part, and (b) is the real part. The inset of (a) shows the quasiparticle density of states (DOS) in the PM and coexisting AFQ/AFM ($T = 6 \times 10^{-3}t$) phase where $\mu = -0.06t$ is the chemical potential. The inset of (b) gives the schematic temperature dependence of order parameters. Quasiparticle model parameters: $t = 22.4$ meV, $\tilde{V} = 0.3t$, and $\tilde{\epsilon}_f = -0.01t$. Gap parameters: $\Delta_{\mathbf{Q}'} = 0.015t$ and $\Delta_{\mathbf{Q}} = 0.005t$ (c) The imaginary part of the RPA susceptibility at the R point (the inset shows the model for the quasiparticle interaction $J_{\mathbf{q}}$ along the ΓR direction, with $J_{\mathbf{Q}'} = 0.1t$).

Fig. 1(a). This explains the central observation of the R-point resonance in CeB_6.

The momentum dependence of the spectrum in the AFQ/AFM phase and, in particular, the resonance peak is shown in Fig. 2 as contour plot in the $\mathbf{q}$, ω plane, with the wave vector $\mathbf{q}$ chosen along various symmetry directions. There are two main characteristics: (i) The single-particle spin gap due to the hybridization and enhanced by the AFQ/AFM gap formation appears most prominently close to the R point and less at other symmetry points like, e.g., $T(\frac{1}{2},\frac{1}{2},\frac{1}{4})$. (ii) The many-body resonance peak is also strongly constrained to the narrow region around the R point, partly due to the suppression of the $\chi_0'(\mathbf{q},\omega)$ peak [Fig. 1(b)] when $\mathbf{q}$ moves away from $R(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ and partly due to the decrease of $J_{\mathbf{q}}$. Both mean that the above condition for the resonance can only be fulfilled in a narrow region around the R point where it is almost dispersionless. This corresponds exactly to the experimental observation in CeB_6, and similar observations have been made in the Ce-based superconductors [18,19]. A complementary constant ω plot of the magnetic scattering intensity which is proportional to $\chi''_{\rm RPA}(\mathbf{q},\omega=\text{const})$ is shown in Fig. 3 for $\mathbf{q}$ in the (hhl) plane as in the experimental scattering geometry. At the resonance position ω_r (a), the momentum-dependent scattering intensity is strongly peaked at the R point with rapid decay in all $\mathbf{q}$ directions into the scattering plane. On the other hand, for $\omega = 0.3\omega_r$ (b), which is in the spin gap region, the latter shows up as a complete depletion of intensity at the R point. Because of the magnetic sum rule, the formation of the spin gap at this energy leads to a roughly even redistribution of the spectral weight across the whole scattering plane. This complete change of constant ω intensity in the (hhl) plane for $\omega = \omega_r$ and $\omega \ll \omega_r$ is in agreement with the experimental result [14].

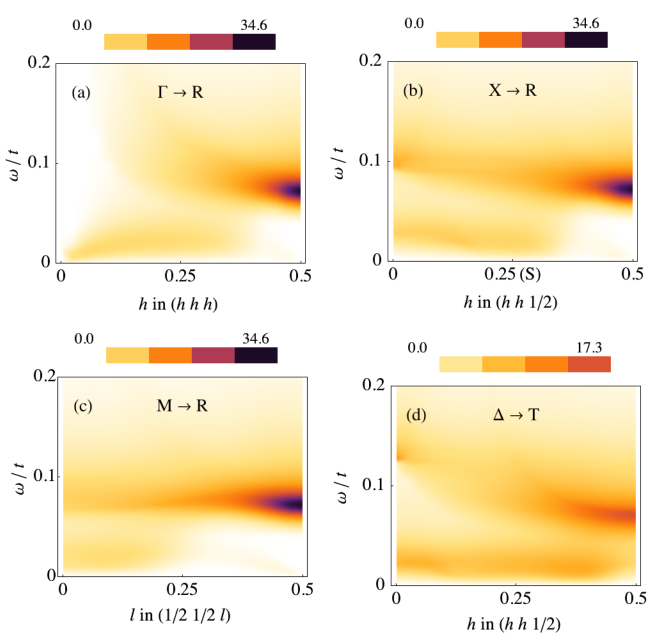

FIG. 2 (color online). Contour plot of the imaginary part of the RPA dynamical susceptibility (a) from $\Gamma(000)$ to $R(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, (b) from $X(00\frac{1}{2})$ to the R point, (c) from the X point to the R point, and (d) from $\Delta(00\frac{1}{2})$ to $T(\frac{1}{2}\frac{1}{2}\frac{1}{4})$ (note the different scale). Resonance is located around R and shows little dispersion.

Now, we discuss the temperature dependence of resonance intensity. We start from itinerant-type AFQ/AFM order parameters in Eq. (2) with a typical MF BCS temperature dependence shown in Fig. 1(b) (inset). The resonance intensity at the HO wave vector in Fig. 1(c) appears already at T_Q and is further enhanced below T_N. Experimentally, it is found that it is strongly suppressed in the region $T_N < T < T_Q$. This is an effect of quadrupole order parameter fluctuations at zero field, due to the near degeneracy with octupole order [24], which strongly suppress its amplitude. For example, the specific heat jump $\Delta C(T_Q)$ for $H = 0$ is almost absent [25], while $\Delta C(T_N)$ is pronounced. However, in finite fields of a few Tesla, the AFQ HO is stabilized and $\Delta C(T_Q, H)$ is strongly enhanced. The stabilization of $\Delta_{\mathbf{Q}'}$ in the field is also directly known from resonant x-ray scattering experiments [7]. This effect will also be present for the dynamical resonance. We therefore predict that the resonance peak at R will appear already in the temperature range $T_N < T < T_Q$ when comparable fields are applied. We note that, even in the case of a single superconducting order parameter, the temperature dependence of the intensity generally deviates from the BCS MF behavior.

In summary, the recent INS experiments [14] require a rethinking of the HO phenomena in CeB_6. The appearance of an itinerant spin exciton resonance at the AFQ wave vector $\mathbf{Q}'$ proves that the previous restriction to localized $4f$ states in CeB_6 for the hidden AFQ order is oversimplified. The neglect of itinerant aspects can no longer be upheld. The theory presented here is therefore built on the delocalized heavy quasiparticle states. They are gapped due to the effect of hybridization and AFQ/AFM-type particle-hole condensation, leading to an enhanced

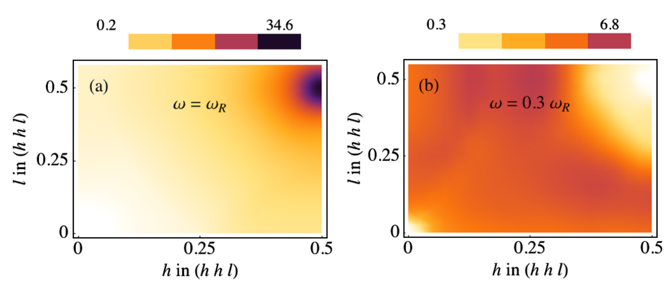

FIG. 3 (color online). Contour plot of the imaginary part of the RPA dynamical susceptibility in the (hhl) plane of the reciprocal space. (a) At $\omega = \omega_r = 0.07t$ (spin exciton resonance energy), a pronounced localized peak at the R point appears (b) for energy in the spin gap, i.e., $\omega = 0.3\omega_r$. Intensity at the R point vanishes due to spin gap formation.

magnetic response at the R point. Because of quasiparticle interaction, a pronounced spin exciton resonance at this wave vector appears. Its salient features of momentum, energy, and temperature dependence are in agreement with experimental observation. Therefore, CeB_6 is the first nonsuperconducting heavy fermion example with a spin exciton resonance excitation originating in the AFQ hidden order state.

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