β-YbAlB_{4}: A Critical Nodal Metal

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β-YbAlB$_4$: a critical nodal metal

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We propose a model for the intrinsic quantum criticality of β-YbAlB$_4$, in which a vortex in momentum space gives rise to a new type of Fermi surface singularity. The unquenched angular momentum of the $|J = 7/2, m_J = \pm 5/2\rangle$ Yb $4f$-states generates a momentum-space line defect in the hybridization between $4f$ and conduction electrons, leading to a quasi-two dimensional Fermi surface with a $k_\perp^4$ dispersion and a singular density of states proportional to $E^{-1/2}$. We discuss the implications of this line-node in momentum space for our current understanding of quantum criticality and its interplay with topology.

Since their discovery, heavy fermion materials have provided a wealth of insights into correlated electron physics. These materials contain a matrix of localized magnetic moments formed from f-electrons immersed in a host metal; at low temperatures the spin-quenching entanglement of the f-moments with the conduction electrons gives rise to a diversity of ground-states, including anisotropic superconductors, Kondo insulators and quasiparticles with effective masses 100s of times that of bare electrons [1, 2]. An important class of heavy fermion metals exhibit the phenomenon of quantum criticality, whereby upon tuning via pressure, doping or magnetic field through a zero temperature 2nd order quantum phase transition, they develop non-Fermi Liquid behavior and predisposition to superconductivity [3–5].

The discovery [6, 7] of an intrinsically quantum critical heavy fermion metal, β-YbAlB$_4$ has recently attracted great interest. β-YbAlB$_4$ exhibits non-Fermi liquid behavior without tuning, with a $T^{3/2}$ temperature dependence of the resistivity and a $T^{-1/2}$ divergence in the magnetic susceptibility; a magnetic field induces an immediate cross-over to a Fermi liquid (FL) with a T^2 resistivity and a susceptibility which diverges as $B^{-1/2}$. T/B scaling in the free energy has been observed over 4 decades of field, pin-pointing the critical magnetic field within ± 0.1 mT of zero and demonstrating that the field-induced Fermi temperature is the Zeeman energy [7].

In this paper, we show that the properties of this material can be understood in terms of a *nodal* hybridization model. In essence β-YbAlB$_4$ resembles a Kondo insulator, but one in which the hybridization gap between the conduction and f-electrons vanishes along a line in momentum space, producing a critical semi-metal with a singular density of states.

There are three known examples of such nodal materials: CeNiSn, CeRhSb and CeCu$_4$Sn, in which the hybridization appears to vanish linearly along a line in momentum space, closing the gap to form a heavy fermion semi-metal [8]. In β-YbAlB$_4$ the unusual local seven-fold symmetry of the ytterbium (Yb) site surrounded by boron (B) atoms protects a "high-spin" $|J = 7/2,\, m_J = \pm 5/2\rangle$ state, in which the f-electrons carry a large unquenched orbital angular momentum. The $|5/2\rangle$ state carries at least two units of unquenched orbital momentum orientated along the c-axis, yet plane waves carry no orbital angular momentum in the direction of motion, so the f-state is protected from hybridization with conduction electrons traveling along the c-axis. This causes the hybridization to develop a singular structure, $V(\mathbf{k}) \sim (k_x \pm i k_y)^2$ vanishing as the square of the transverse momentum $\mathbf{k}_\perp$ with a double-vorticity associated with the two unquenched units of orbital angular momentum. The electrons and holes at the band-edge then form an emergent two-dimensional electron gas with a dispersion proportional to the square of the hybridization,

$$E(\mathbf{k}) \sim |V(\mathbf{k})|^2 \sim (k_\perp)^4, \tag{1}$$

giving rise to a quartic dispersion with a divergent density of states $N(E) \propto E^{-1/2}$. It is the field-induced doping of this two-dimensional heavy band that accounts for the unusual field-tuned behavior in β-YbAlB$_4$.

In β-YbAlB$_4$ the Yb atoms form a honeycomb lattice, sandwiched between layers of B atoms, with the Yb atoms sitting between a pair of 7-member B rings, giving rise to a local environment with local seven-fold symmetry [6], as shown in Fig. 1. We shall assume that the Yb ions are in a nominal Yb^{3+}, $4f^{13}$ configuration, with total angular momentum $J = 7/2$. Photoemission spectroscopy indicates a microscopic valence of 2.75 [9] due to moment-conserving valence fluctuations $Yb^{3+} \leftrightarrow Yb^{2+} + e^-$.

J=7/2 crystal field operators with 7-fold and time-reversal symmetries conserve total J_z, splitting the J=7/2 Yb multiplet into four Kramers doublets, each with definite $|m_J|$. The Curie constant and the Ising anisotropy of the magnetic susceptibility of β-YbAlB$_4$ are consistent with a pure Yb ground-state doublet $|J = 7/2, m_J = \pm 5/2\rangle$ [10], a configuration that ex-

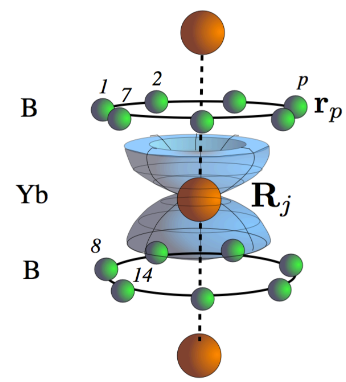

FIG. 1. Showing the seven-fold symmetric environment of the Yb^{3+} ions (large spheres) in β-$YbAlB_4$, sandwiched between two heptagonal rings of B atoms (small spheres). The blue surface is the orbital distribution in the $m_j = \pm 5/2$ state.

hibits maximal hybridization with the seven-fold boron rings. This Ising ground-state is also consistent with the large anisotropic g-factor observed in electron spin resonance measurements on β-$YbAlB_4$ [11].

We model the low energy physics of β-$YbAlB_4$ as a layered Anderson lattice [10],

$$H = \sum_{n,k,\sigma} \epsilon_{\mathbf{k}n} c^\dagger_{\mathbf{k}n\sigma} c_{\mathbf{k}n\sigma} + \sum_j H_m(j), \tag{2}$$

where the first term describes a tight-binding boron conduction electron band with index n, and

$$H_m(j) = V_0(c^\dagger_{j\alpha} X_{0\alpha}(j) + \text{h.c.}) + E_f X_{\alpha\alpha}(j), \tag{3}$$

describes the hybridization with the Yb ion at site j and the energy level E_f of the f-electrons. Here, $X_{0\alpha} = |4f^{14}\rangle\langle 4f^{13}, \alpha|$ is a Hubbard operator linking the $4f^{13}$, $m_J \equiv \alpha = \pm 5/2$ state of the Yb^{3+} ion to the completely filled shell Yb^{2+} state $|4f^{14}\rangle$. The operator

$$c^\dagger_{j\alpha} = \sum_{p\in(1,14),\sigma} c^\dagger_\sigma(\mathbf{R}_{jp})\, \mathcal{Y}_{\sigma\alpha}(\mathbf{r}_p), \tag{4}$$

creates a conduction electron in a Wannier state delocalized across the seven-fold boron rings directly above and below the Yb ion at site j, with local f symmetry and $J_z = \alpha = \pm 5/2$. The $\mathbf{R_{jp}} = \mathbf{R_j} + \mathbf{r_p}$ are the locations of the fourteen boron sites around the Yb site j (see Fig. 1). The hybridization matrix,

$$\mathcal{Y}_{\sigma\alpha}(\mathbf{r}) = C^{\frac{7}{2}}_{\sigma\alpha} Y^3_{\alpha-\sigma}(\mathbf{r}) = \frac{1}{\sqrt{7}} \begin{pmatrix} \sqrt{6}Y^3_2 & Y^3_3 \\ Y^3_{-3} & \sqrt{6}Y^3_{-2} \end{pmatrix} (\hat{\mathbf{r}}), \tag{5}$$

where the $C^{\frac{7}{2}}_{\sigma\alpha} = \langle 3\alpha - \sigma, \frac{\sigma}{2} | \frac{7}{2}, \alpha\rangle$ are Clebsch-Gordan coefficients for the Yb^{3+}, $\alpha = \pm 5/2$ configurations.

We employ a slave boson decomposition of the Hubbard operators, $X_{0\alpha}(j) = b^\dagger_j f_{j\alpha}$, where b_j and $f_{j\alpha}$ are a slave boson and an Abrikosov pseudo-fermion respectively; in a mean-field approximation,

$$H_m(j) = V_0^*[c^\dagger_{j\alpha} f_{j\alpha} + \text{h.c.}] + \tilde{E}_f f^\dagger_{j\alpha} f_{j\alpha} + \lambda_0(r^2 - 1), \tag{6}$$

where V_0^* is the quasiparticle hybridization, renormalized by the mean-field amplitude of the slave boson field, $r = |\langle b\rangle|$ taken to be constant at each site. λ_0 imposes the mean-field constraint $\langle n_f\rangle + r^2 = 1$, while the renormalized position of the f-level $\tilde{E}_f = \lambda_0 + E_f$.

Next, we transform to momentum space and evaluate the form-factor of the seven-fold symmetric Yb-B cluster. To obtain a simplified model, let us assume a single band of dispersion $\epsilon_{\mathbf{k}}$ hybridizing with the Yb atom. Rewriting the creation operator at a given boron site in terms of a plane wave state $c^\dagger_\sigma(\mathbf{R}_{jp}) = (4\mathcal{N})^{-1/2}\sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{R}_{jp}}$, and $f_{j\alpha} = \mathcal{N}^{-1/2}\sum_{\mathbf{k}} f_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{R}_j}$ where $\mathcal{N}$ is the number of Yb sites, Eq. (4) becomes:

$$c^\dagger_{j\alpha} = (4\mathcal{N})^{-1/2} \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} \gamma_{\sigma\alpha}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_j},$$

where the form-factor of the Yb-B cluster

$$[\underline{\gamma}(\mathbf{k})]_{\sigma\alpha} = \sum_{p=1,14} \mathcal{Y}_{\sigma\alpha}(\mathbf{r}_p) e^{-i\mathbf{k}\cdot\mathbf{r}_p}. \tag{7}$$

The mean-field Hamiltonian (6) can then be written in terms of the plane-wave $c_{\mathbf{k}\sigma}$ and $f_{\mathbf{k}\alpha}$ operators as

$$H_{eff} = \sum_{\mathbf{k}} (c^\dagger_{\mathbf{k}}, f^\dagger_{\mathbf{k}}) \begin{pmatrix} \epsilon_{\mathbf{k}}\mathbb{I} & \underline{V}(\mathbf{k}) \\ \underline{V}^\dagger(\mathbf{k}) & \tilde{E}_f\mathbb{I} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}} \\ f_{\mathbf{k}} \end{pmatrix}, \tag{8}$$

where all details of the hybridization are hidden in the matrix $[\underline{V}(\mathbf{k})] = \frac{1}{2}V_0^*\underline{\gamma}(\mathbf{k})$. Now in polar co-ordinates

$$\mathcal{Y}(\hat{\mathbf{r}}) = \sqrt{\frac{5}{64\pi}}\, s_\theta^2 \begin{pmatrix} 6c_\theta e^{2i\phi} & -s_\theta e^{3i\phi} \\ s_\theta e^{-3i\phi} & 6c_\theta e^{-2i\phi} \end{pmatrix}, \tag{9}$$

where we denote $(\cos\theta, \sin\theta) \equiv (c_\theta, s_\theta)$. The important point, is that the hybridization vanishes as $\sin^2\theta$ along the c-axis. Now the effect of Fourier transforming in Eq. (7), is to replace the real-space argument by the momentum $\mathcal{Y}(\mathbf{r}) \to \mathcal{Y}(\mathbf{k})$. To obtain an analytic expression, we approximate the discrete sum over the positions in the seven-fold B ring by a continuous integral: $\sum_p \to 7\sum_\pm \int \frac{d\phi}{2\pi}$. We find that $V(\mathbf{k})$ is proportional to a unitary matrix,

$$V(\mathbf{k}) = i\tilde{V}_0 \begin{pmatrix} \alpha_{\mathbf{k}} & \beta_{\mathbf{k}} \\ -\beta^*_{\mathbf{k}} & \alpha^*_{\mathbf{k}} \end{pmatrix}, \tag{10}$$

where $\tilde{V}_0 = \frac{7V_0^*}{16}\sqrt{\frac{5}{\pi}}$ and

$$\begin{aligned} \alpha_{\mathbf{k}} &= 6\sin(k_z a/2)(\hat{k}_x + i\hat{k}_y)^2 J_2(k_\perp R) \\ \beta_{\mathbf{k}} &= \cos(k_z a/2)(\hat{k}_x + i\hat{k}_y)^3 J_3(k_\perp R), \end{aligned} \tag{11}$$

where J_n are Bessel functions of order n, R is the radius of the seven-fold rings and a is the distance between boron layers. Since $J_n(x) \propto x^n$ at small x, near the c-axis, the hybridization vanishes as $k_\perp^2$, with a diagonal form

$$V(\mathbf{k}) \sim \begin{pmatrix} (k_x + ik_y)^2 & 0 \\ 0 & (k_x - ik_y)^2 \end{pmatrix}.$$

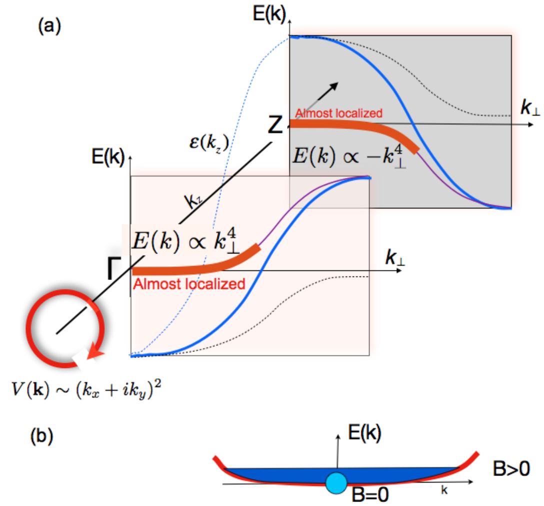

FIG. 2. (a) Showing dispersion around the c-axis, with an electron pocket at the Γ point and a hole pocket at the Z point. (b) Magnetic field fills the $k_\perp^4$ band.

As one proceeds around the c-axis, the phase of the hybridization advances by 4π, forming a double vortex in the hybridization along the c-axis. This *vorticity* is a consequence of angular momentum conservation about the c-axis: plane waves $|\mathbf{k}\sigma\rangle$ traveling along the c-axis carry a spin angular momentum of $\pm\frac{1}{2}$ along the c-axis, and because the f-states are in an $m_J = \pm\frac{5}{2}$, angular momentum conservation prevents the mixing of conduction and f-electron waves travelling along the c-axis.

We can diagonalize the mean-field Hamiltonian, to obtain a hybridized dispersion

$$E^\pm_{\mathbf{k}} = \frac{1}{2}(\epsilon_{\mathbf{k}} + \tilde{E}_f) \pm \left[\frac{1}{4}(\epsilon_{\mathbf{k}} - \tilde{E}_f)^2 + |V(k)|^2\right]^{\frac{1}{2}}, \quad (12)$$

where $|V(k)|^2 = \tilde{V}_0^2[|\alpha_{\mathbf{k}}|^2 + |\beta_{\mathbf{k}}|^2]$. Fig. 2 illustrates the hybridized band-structure. Near the c-axis, the squared hybridization vanishes as $V(\mathbf{k})^2 = A(k_z)k_\perp^4$. The dispersion in the vicinity of the c-axis is then given by

$$E(k_\perp, k_z) = \tilde{E}_f + \frac{V(\mathbf{k})^2}{-\epsilon(k_z)} \approx \tilde{E}_f + \eta(k_z)k_\perp^4.$$

where $\eta(k_z) = \frac{A(k_z)}{-\epsilon(k_z)}$ and we have assumed that $|\epsilon(k_z)|$ is large compared to $|V(k)|$. In other words, the system develops an emergent two-dimensional Fermi surface, with a $k_\perp^4$ dispersion. A hole band is formed in the region where $\epsilon(k_z) > 0$, while an electron band is formed in the region where $\epsilon(k_z) < 0$. In the case where $\epsilon(k_z)$ changes sign along the c-axis, a two dimensional electron and hole band is formed above and below the f-level.

To explain the intrinsic criticality of β-$YbAlB_4$ we conjecture that the f-level is pinned to zero energy $\tilde{E}_f = 0$. A heuristic argument for this assumption, is to regard β-$YbAlB_4$ as a Kondo insulator in which the nodal hybridization closes the gap along the c-axis, pinching the f-level in the gap at precisely zero energy. At the current stage of understanding, this assumption is purely phenomenological, a point we return to later.

If $\tilde{E}_f = 0$, the density of states for this dispersing system is then given by $N^*(E) = \sum_\pm N^*_\pm(E)\theta(\pm E)$, where

$$N^*_\pm(E) = 2\int k_\perp \frac{dk_\perp}{dE_\pm}\frac{dk_z}{(2\pi)^2} = \frac{1}{\sqrt{|E|T_0^\pm}} \quad (13)$$

and $\frac{1}{\sqrt{T_0^\pm}} = \frac{1}{8\pi^2}\int \frac{dk_z}{\sqrt{|\eta(k_z)|}}\theta[\mp\epsilon(k_z)]$ determines the characteristic scales $T_0^\pm$ for the electron (+) and hole (-) branch of the dispersion. Powerlaw scaling will extend out to characteristic Kondo temperature T_K of the system, so that the total weight x of f-electrons contained within the divergent peak is $2x = \int_{-T_K}^{T_K} N^*(E) \approx 4\sqrt{T_K/T_0}$, giving $T_0 = 4T_K/x^2$.

If the f-level is pinned to zero energy, then at low temperatures a Fermi line of zero energy excitations forms along the c-axis. In a field, the Zeeman-splitting of the f-level induces a singular polarization of nodal electron and hole bands, broadening the Fermi line into a distinct tubular Fermi surface. When a field is introduced, a spin-polarized Fermi surface grows around the line-zero in the hybridization, giving rise to a density of states of order $N^*[\frac{g}{2}\mu_B B] \sim B^{-1/2}$, leading to a Pauli susceptibility that diverges as $\chi \sim B^{-1/2}$. We call this field-induced Fermi surface transition a "vortex transition". Vortex transitions are reminiscent of a Lifshitz transition, but whereas Lifshitz transitions are point defects in momentum space [12, 13], the vortex transition is a line defect.

We can model the singular thermodynamics of the system with the Free energy

$$\begin{aligned} F[B,T] &= -T\sum_{\alpha=\pm 5/2}\int_{-\infty}^{\infty} dE N(E)\ln[1+e^{-\beta(E-g\mu_B B\alpha)}] \\ &= T^{3/2}\Phi\left(\frac{g\mu_B B}{T}\right) \end{aligned} \quad (14)$$

where

$$\Phi(y) = -\frac{1}{\sqrt{T_0}}\int_0^\infty \frac{dx}{\sqrt{|x|}}\sum_{\alpha=\pm 5/2}\ln[1+e^{-x-y\alpha}]$$

and $T_0^{-1/2} = (1/2)\sum_\pm T_\pm^{-1/2}$. Fig. 3 compares the experimental scaling curve [7] with that predicted by our simple model. However, while a qualitatively good fit to the observations is obtained using a gyromagnetic ratio consistent with the single ion properties of Yb in β-$YbAlB_4$, the characteristic energy scale required to fit the experimental results is $T_0 \sim 6.5eV$, far greater than the characteristic Kondo temperature ($\sim 200K$) of this system [7]. Using our relationship $T_0 = 4T_K/x^2$, we can understand this scale by assuming that about $x \sim 0.1$ of the f-spectral weight is contained within the vortex metal contribution to the density of states.

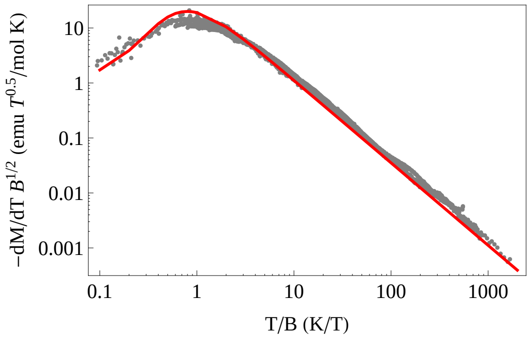

FIG. 3. Theoretical fit (red line) to the measured field-dependent magnetization of β-YbAlB_4 from [7] (gray dots) using formula 14 with $gm_J = 2.85$ and $T_0 = 6.65eV$.

We now turn to discuss some of the assumptions behind our model. One issue is whether the plane-wave description of the vortex metal survives inclusion of band-structure effects. In this situation, angular momentum is only conserved modulo n$\hbar$, where n is the order of the symmetry group of the Yb environment, requiring $n \geq 5$ to avoid any admixture of $|m_J| = 3/2, 1/2$ states into the perfect $\pm 5/2$ doublet. In a model of β-YbAlB_4 , using tight-binding coupling within the B planes and perfect heptagonal Yb rings, the nodal structure does indeed survive, as shown in Fig. 4. However more work is required to understand whether the nodes persist in a more realistic model of β-YbAlB_4 . Another key assumption is that the pinching of the hybridization gap by the node perfectly pins the f-level to the Fermi surface. Ultimately, this must arise from Coulomb screening, an effect that also needs inclusion in future work.

Support for our model is provided by the locally isostructural polymorph $\alpha-$YbAlB_4, which has a comparable characteristic "Kondo" scales $T_K \approx 200K$ [9] to the beta phase, but develops a FL ground state [14]. Recent experiments indicate that α-YbAlB_4 develops a two dimensional Fermi liquid at fields $B > 3T$ [15], suggesting it is a phase in which the f-level has become detached from the Fermi energy. More direct confirmation of our nodal hybridization model of β-YbAlB_4 might be obtained from de Haas-van Alphen measurements. Using Onsager's arguments, the free energy of an extremal orbit of area A_{FS} in the field-doped FL will be a periodic function of $\hbar A_{FS}/(2\pi e B)$, and since $A_{FS} \propto \sqrt{B}$, unlike conventional metals, we predict the low-field quantum oscillations will be periodic in $1/\sqrt{B}$ rather than $1/B$.

Finally, we note that vortex structure in the hybridization suggests a kind of topological line defect in momentum space. In Kondo insulators, the hybridization vanishes at the high symmetry points forming point defects [12], corresponding to a homotopy $\Pi_2(\mathcal{H}) = \mathbb{Z}_2$. Vortices in the hybridization suggest a further one dimensional homotopy, $\Pi_1(H) = \mathbb{Z}$. This is an interesting direction for future work.

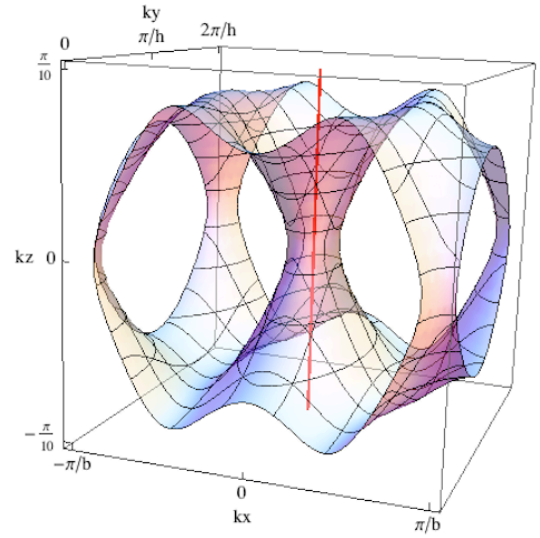

FIG. 4. Fermi surface from a tight-binding calculation. Note the cylindrical feature along the z-axis linked to an almost 2D surface in the $k_x - k_y$ plane. For clarity, the 1st BZ has been shifted by π/h to move the node into the center of the zone.

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