Cubic Topological Kondo Insulators

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\textbf{Dated: February 7, 2014}

Current theories of Kondo insulators employ the interaction of conduction electrons with localized Kramers doublets originating from a tetragonal crystalline environment, yet all Kondo insulators are cubic. Here we develop a theory of cubic topological Kondo insulators involving the interaction of $\Gamma_8$ spin quartets with a conduction sea. The spin quartets greatly increase the potential for strong topological insulators, entirely eliminating the weak-topological phases from the diagram. We show that the relevant topological behavior in cubic Kondo insulators can only reside at the lower symmetry X or M points in the Brillouin zone, leading to three Dirac cones with heavy quasiparticles.

PACS numbers: 72.15.Qm, 73.23.-b, 73.63.Kv, 75.20.Hr

Our classical understanding of order in matter is built around Landau’s concept of an order parameter. The past few years have seen a profound growth of interest in topological phases of matter, epitomized by the quantum Hall effect and topological band insulators, in which the underlying order derives from the non-trivial connectedness of the quantum wave-function, often driven by the presence of strong spin-orbit coupling \cite{1–9}.

One of the interesting new entries to the world of topological insulators, is the class of heavy fermion, or “Kondo insulators” \cite{10–16}. The strong-spin orbit coupling and highly renormalized narrow bands in these intermetallic materials inspired the prediction \cite{12} that a subset of the family of Kondo insulators will be $Z_2$ topological insulators. In particular, the oldest known Kondo insulator SmB$_6$\cite{17} with marked mixed valence character, was identified as a particularly promising candidate for a strong topological insulator (STI): a conclusion that has since also been supported by band-theory calculations \cite{13, 16}. Recent experiments \cite{18–20} on SmB$_6$ have confirmed the presence of robust conducting surfaces, large bulk resistivity and a chemical potential that clearly lies in the gap providing strong support for the initial prediction.

However, despite these developments, there are still many aspects of the physics in these materials that are poorly understood. One of the simplifying assumptions of the original theory \cite{12} was to treat the $f$-states as Kramer’s doublets in a tetragonal environment. In fact, the tetragonal theory predicts that strong topological insulating behavior requires large deviations from integral valence, while in practice Kondo insulators are much closer to integral valence \cite{11}. Moreover, all known Kondo insulators have cubic symmetry, and this higher symmetry appears to play a vital role, for all apparent “Kondo insulators” of lower symmetry, such as CeNiSn\cite{21} or CeRu$_4$Sn$_6$\cite{22} have proven, on improving sample quality, to be semi-metals. One of the important effects of high symmetry is the stabilization of magnetic $f$-quartets. Moreover, Raman\cite{23} experiments and various band-theory studies\cite{24, 25} that it is the Kondo screening of the magnetic quartets that gives rise to the emergence of the insulating state.

Motivated by this observation, here we formulate a theory of cubic topological Kondo insulators, based on a lattice of magnetic quartets. We show that the STI phase extends into the Kondo limit. For SmB$_6$ $\nu = 3 - n_f$ gives the valence of the Sm ion, while $n_f$ measures the number of $f$-holes in the filled $4f^6$ state, so that $n_f = 1$ corresponds to the $4f^5$ configuration.

![FIG. 1: Contrasting the phase diagram of tetragonal and cubic topological Kondo insulators.](image-url)
zone (BZ), leading to a three heavy Dirac cones at the surface. One of the additional consequences of the underly-
ing Kondo physics, is that the coherence length of the surface states is expected to be very small, of order a lattice spacing.

While we outline our model of cubic Kondo insulators with a particular focus on SmB$_6$, the methodology generalizes to other cubic Kondo insulators. SmB$_6$ has a simple cubic structure, with the B$_6$ clusters located at the center of the unit cell, acting as spacers which mediate electron hopping between Sm sites. Band-theory [24] and XPS studies [23] show that the 4f orbitals hybridize with d-bands which form electron pockets around the X points. In a cubic environment, the $J = 5/2$ orbitals split into a $\Gamma_7$ doublet and a $\Gamma_8$ quartet, while the fivefold degenerate d-orbitals are split into double degenerate $e_g$ and triply degenerate $t_{2g}$ orbitals. Band theory and Raman spectroscopy studies [23] indicate that the physics of the 4f orbitals is governed by valence fluctuations involving electrons of the $\Gamma_8$ quartet and the conduction $e_g$ states, $e^{-} + 4f^5(\Gamma_8^{(1)}) \rightleftharpoons 4f^6$. The $\Gamma_8^{(1)} (a = 1, 2)$ quartet consists of the following combination of orbitals:

$$|\Gamma_8^{(1)}\rangle = \sqrt{\frac{5}{6}}|\pm \frac{1}{2}\rangle + \sqrt{\frac{1}{6}}|\pm \frac{3}{2}\rangle, \quad |\Gamma_8^{(2)}\rangle = |\pm \frac{1}{2}\rangle.$$  

This then leads to a simple physical picture in which the $\Gamma_8$ quartet of f-states hybridizes with an $e_g$ quartet (Kramers plus orbital degeneracy) of d-states to form a Kondo insulator.

To gain insight into how the cubic topological Kondo insulator emerges it is instructive to consider a simplified one-dimensional model consisting of a quartet of conduction d-bands hybridized with a quartet of f-bands (Fig. 2a). In one dimension there are two high symmetry points: $\Gamma$ ($k = 0$) and X ($k = \pi$), where the hybridization vanishes [12, 14, 26]. Away from the zone center $\Gamma$, the f− and d−quartets split into Kramers doublets. The $Z_2$ topological invariant $\nu_{1D}$ is then determined by the product of the parities $\nu_{1D} = \delta_{\Gamma} \delta_{X}$ of the occupied states at the $\Gamma$ and X points. However, the f-quartet at the $\Gamma$ point is equivalent to two Kramers doublets, which means that $\delta_{\Gamma} = (\pm 1)^2$ is always positive, so that $\nu_{1D} = \delta_{X}$ and a one-dimensional topological insulator only develops when the f and d bands invert at the X point.

Generalizing this argument to three dimensions we see that there are now four high symmetry points $\Gamma$, X, M and R. The f-bands are fourfold degenerate at both $\Gamma$ and R points which guarantees that $\delta_{\Gamma} = \delta_{R} = +1$ (Fig. 2b). Therefore, we see that the 3D topological invariant is determined by band inversions at X or M points only, $\nu_{3D} = (\delta_{X} \delta_{M})^3 = \delta_{X} \delta_{M}$. If there is a band inversion at the X point, we get $\nu_{3D} = \delta_{X} \delta_{M} = -1$. In this way the cubic character of the Kondo insulator and, specifically, the fourfold degeneracy of the f-orbital multiplet protects the formation of a strong topological insulator.

We now formulate our model for cubic topological Kondo insulators. At each site, the quartet of f and d−holes is described by an orbital and spin index, denoted by the combination $\lambda \equiv (a, \sigma)$ ($a = 1, 2, \sigma = \pm 1$). The fields are then given by the eight component spinor

$$\Psi_{j} = \begin{pmatrix} d_{\lambda}(j) \\ X_{0\lambda}(j) \end{pmatrix}$$  

where $d_{\lambda}(j)$ destroys an d-hole at site j, while $X_{0\lambda}(j) = |4f^0\rangle|4f^1\rangle, \lambda|$ is the the Hubbard operator that destroys an f-hole at site j. The tight-binding Hamiltonian describing the hybridized f−d system is then

$$H = \sum_{i,j} \Psi_{j}^\dagger(i)h_{\lambda\lambda'}(R_i - R_j)\Psi_{j'}(j)$$  

in which the nearest hopping matrix has the structure

$$h_{\lambda}(R) = \begin{pmatrix} h^d(R) & V^\dagger(R) \\ V(R) & h^f(R) \end{pmatrix},$$  

where the diagonal elements describe hopping within the d− and f−quartets while the off-diagonal parts describe the hybridization between them, while $R \in \{\pm \hat{x}, \pm \hat{y}, \pm \hat{z}\}$ is the vector linking nearest neighbors. The various matrix elements simplify for hopping along the z-axis, where they become orbital and spin diagonal:

$$h^l(z) = t^l \begin{pmatrix} 1 & \eta_l \\ \eta_l & 0 \end{pmatrix}, \quad V(z) = i V \begin{pmatrix} 0 \\ \sigma_z \end{pmatrix},$$  

where $l = d, f$ and $\eta_l$ is the ratio of orbital hopping elements. In the above, the overlap between the $\Gamma_8^{(1)}$ orbitals, which extend perpendicular to the z-axis is neglected, since the hybridization is dominated by the overlap of the the $\Gamma_8^{(2)}$ orbitals, which extend out along the z-axis. The hopping matrix elements in the $x$ and $y$ directions are then obtained by rotations in orbital/spin
space. so that \( h(x) = U_y h(z) U_y^\dagger \) and \( h(y) = U_{-x} h(z) U_{-x}^\dagger \), where \( U_y \) and \( U_{-x} \) denote 90° rotations about the y and negative x axes, respectively.

The Fourier transformed hopping matrices \( h(k) = \sum_{\mathbf{R}} h(\mathbf{R}) e^{-i k \cdot \mathbf{R}} \) can then be written in the compact form

\[
h'_l(k) = t'_l \left( \phi_1(k) + \eta_l \phi_2(k) \right) \left( 1 - \eta_l \right) \phi_3(k) + \phi_l(k) \right) + \epsilon', \quad (5)
\]

where \( l = d, f \). Here \( \epsilon' \) are the bare energies of the isolated d and f-quartets, while \( \phi_1(k) = e_x + e_y + 4e_z, \quad \phi_2(k) = 3(e_x + e_y) \) and \( \phi_3(k) = \sqrt{3}(e_x - e_y) \) \( (e_a \cos k_a, \alpha = x, y, z) \). The hybridization is given by

\[
V(k) = \frac{1}{6} \left( 3(\sigma_x + i\sigma_y) \sqrt{3} \sigma_x - i\sigma_y \right) \sigma_x + i\sigma_y + 4\sigma_z \right)
\]

where we denote \( \sigma_a = \sigma_a \sin k_a \). Note how the hybridization between the even parity d-states and odd-parity f-states is an odd parity function of momentum \( V(k) = -V(-k) \).

To analyze the properties of the Kondo insulator, we use a slave boson formulation of the Hubbard operators, writing \( X_\alpha \phi_\lambda = f_\lambda^z(0) \phi_\lambda \), where \( f_\lambda^z(0) \equiv |4f^{0,\lambda}, \phi_\lambda \) creates an f-hole in the \( \Gamma^8 \) quartet while \( b_\lambda^\dagger(0) \equiv |4f^{0,\lambda}, \phi_\lambda \) denotes the singlet filled 4f shell, subject to the constraint \( Q_j = b_j^\dagger b_j + \sum_\lambda f_\lambda^z j f_\lambda^\dagger = 1 \) at each site.

FIG. 3: Temperature dependence of the hybridization gap parameter \( b \) and the renormalized f-level position (inset) for various values of the bare hybridization (see Supplementary Materials for more details).

We now analyze the properties of the cubic Kondo insulator, using a mean-field treatment of the slave boson field \( b_i \), replacing the slave-boson operator \( b_i \) at each site by its expectation value: \( \langle b_i \rangle = b \) so that the f- hopping and hybridization amplitude are renormalized: \( t_f \rightarrow b^2 t_f \) and \( V_{df} \rightarrow bV_{df} \). The mean-field theory is carried out, enforcing the constraint \( b^2 + \langle n_f \rangle = 1 \) on the average. In addition, the chemical potentials \( \epsilon_d \) and \( \epsilon_f \) for both d-electrons and f-holes are adjusted self-consistently to produce a band insulator, \( n_d + n_f = 4 \). This condition guarantees that four out of eight doubly degenerate bands will be fully occupied. The details of our mean-field calculation are given in the Supplementary Materials section. Here we provide the final results of our calculations.

In Fig. 3 we show that the magnitude \( b \) reduces with temperature, corresponding to a gradual rise in the Sm valence, due to the weaker renormalization of the f-electron level. The degree of mixed valence of Sm\(^{+}\) is given then by \( v = 3 - (n_f) \). In our simplified mean-field calculation, the smooth temperature cross-over from Kondo insulating behavior to local moment metal at high temperatures is crudely approximated by an abrupt second-order phase transition.

FIG. 4: Band structure consistent with PES and LDA studies of SmB\(_6\) computed with the following parameters: \( n_f = 0.48 \) \( (or b = 0.73), V = 0.05 \text{ eV}, t_d = 2 \text{ eV}, \mu_d = 0.2 \text{ eV}, \eta = \eta' = -3, \epsilon_f = -0.01 \text{ eV} (\epsilon_{f0} = -0.17 \text{ eV}), t_f = -0.05 \text{ eV}, T = 10^{-4} \text{ eV} \) and the gap is \( \Delta = 12 \text{ meV} \). Shaded region denotes filled bands. Inset shows the ground-state energy computed for a slab of 80 layers to illustrate the three gapless surface Dirac excitations at the symmetry points \( \Gamma, X' \text{and} X'' \).

FIG. 4 shows the computed band structure for the cubic Kondo insulator obtained from mean-field theory, showing the band inversion between the d- and f-bands at the X points that generates the strong topological insulator. Moreover, as the value of the bare hybridization increases, there is a maximum value beyond which the bands no longer invert and the Kondo insulator becomes a conventional band insulator.

One of the interesting questions raised by this work concerns the many body character of the Dirac electrons on the surface. Like the low-lying excitations in the valence and conduction band, the surface states of a TKI involve heavy quasiparticles of predominantly f-character. The characteristic Fermi velocity of these excitations \( v_F^* = Z v_F \) is renormalized with respect to the conduction electron band group velocities, where \( Z = m/m^* \) is the mass renormalization of the f-electrons. In a band topological insulator, the penetration depth of the sur-
face states $\xi \sim v_F/\Delta$, where $\Delta$ is the band-gap, scale that is significantly larger than a unit-cell size. Paradoxically, even though the Fermi velocity of the Dirac cones in a TKI is very low, we expect the characteristic penetration depth $\xi$ of the heavy wavefunctions into the bulk to be of order the lattice spacing $a$. To see this, we note that $\xi \sim \sqrt{\frac{\hbar}{2m\Delta}}$, where the indirect gap of the Kondo insulator $\Delta_\parallel$ is of order the Kondo temperature $\Delta_\parallel \sim T_K$. But since $T_K \sim ZW$, where $W$ is the width of the conduction electron band, this implies that the penetration depth of the surface excitations $\xi \sim v_F/W \sim a$ is given by the size $a$ of the unit cell. Physically, we can interpret the surface Dirac cones as a result of broken Kondo singlets, whose spatial extent is of order a lattice spacing. This feature is likely to make the surface states rather robust against the purity of the bulk.

Various interesting questions are raised by our study. Conventional Kondo insulators are most naturally understood as a strong-coupling limit of the Kondo lattice, where local singlets form between a commensurate number of conduction electrons and localized moments. What then is the appropriate strong coupling description of topological Kondo insulators, and can we understand the surface states in terms of broken Kondo singlets? A second question concerns the temperature dependence of the hybridization gap. Experimentally, the hybridization gap observed in Raman studies is seen to develop in a fashion strongly reminiscent of the mean-field theory. Could this indicate that fluctuations about mean-field theory are weaker in a fully gapped Kondo lattice than the predicted three Dirac cones. These ground-state of the f-state a Kramers doublet, then we would expect a single Dirac cone excitation. These consequences of the quartet model is the prediction of enhanced effective mass. By contrast, were the underlying state states in terms of broken Kondo singlets, whose spatial extent is of order a lattice spacing. This feature is likely to make the surface states rather robust against the purity of the bulk.

We end with a few comments on the experimental consequences of the above picture. One of the most dramatic consequences of the quartet model is the prediction of three Dirac cones of surface excitation of substantially enhanced effective mass. By contrast, were the underlying state states in terms of broken Kondo singlets, whose spatial extent is of order a lattice spacing. This feature is likely to make the surface states rather robust against the purity of the bulk.

We would like to thank A. Ramires, V. Galitski, K. Sun, S. Artyukhin and J. P. Paglione for stimulating discussions related to this work. This work was supported by the Ohio Board of Regents Research Incentive Program grant OBR-RIP-220573 (M.D.), DOE grant DE-FG02-99ER45790 (V. A & P. C.), the U.S. National Science Foundation I2CAM International Materials Institute Award, Grant DMR-0844115.

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SUPPLEMENTARY MATERIALS FOR CUBIC TOPOLOGICAL KONDO INSULATORS

These notes provide:

- details of the derivation of the tight-binding Hamiltonian for a cubic Kondo insulator.
- derivation of the mean-field theory for the infinite $U$ limit
- derivation of the mean-field equations.

Rotation matrices

To construct the Hamiltonian, we evaluate the hopping matrices along the $z$-axis, and then carry out a unitary transformation to evaluate the corresponding quantities for hopping along the $x$ and $y$ axes.

Consider a general rotation operator

$$\mathcal{R} = R\Lambda,$$

where $R$ and $\Lambda$ describe $\pi/2$ rotations about a principle axis of the crystal in real and spin space respectively. The Hamiltonian in a cubic environment is invariant under these transformations: $H = \mathcal{R}^\dagger H \mathcal{R}$. We now write the directional dependence of the Hamiltonian explicitly.

$$H(x, y, z) = (RA)^\dagger H(x, y, z)R\Lambda = \Lambda^\dagger (R^\dagger H(x, y, z)R)\Lambda.$$  

We can always choose the rotation $\mathcal{R}$ to transform in the cyclic manner: $x \rightarrow y \rightarrow z \rightarrow x$, then substituting $z = y = 0$,

$$H(x, 0, 0) = \Lambda^\dagger (R^\dagger H(x, 0, 0)R)\Lambda = \Lambda^\dagger H(0, 0, x)\Lambda,$$

hence we can assume the 3D Hamiltonian of the following form

$$H_{3D} = H(k_z) + \Lambda H(k_x)\Lambda^\dagger + \Lambda^\dagger H(k_y)\Lambda,$$

Where to rotate in the opposite direction we use $\Lambda^{-1} = \Lambda^\dagger$. Using the Wigner D-functions we can construct the rotation in angular momentum space

$$\Lambda = e^{-i\alpha J_x}e^{-i\beta J_y}e^{-i\gamma J_z}.$$  

Here, $\Lambda$ denotes the rotation operator in the "ZYX" convention, corresponding to a rotation around the $z$-axis, followed by a rotation around the $y$-axis, and then the new $z$-axis. The matrix elements of this operator are then

$$D^J_{m'm} = \langle Jm' | \Lambda | Jm \rangle$$

$$= \left[ (j + m)!(j - m)!(j + m')!(j - m')! \right]^{1/2}$$

$$\times \sum_{\chi} \frac{(\chi^J \chi^{J'})^{-1/2} \chi^{J'} \chi^{J'}} \chi^{m'-m} \chi^{m-m'}$$

$$\times \left( \cos \frac{\beta}{2} \right)^{2j+m-m'-2\chi} \left( -\sin \frac{\beta}{2} \right)^{m'-m+2\chi} e^{-i\alpha \chi - i\gamma \chi},$$

so that upon rotating the state $|Jm\rangle$ using $R_x$ we obtain $\Lambda^{(j=5/2)} = D_{mn,\omega}^{5/2}(0, \pi/2, \pi/2)$, and $\Lambda^{(j=2)} = D_{mn,\omega}^2$ etc. One can now obtain the transformation matrices for a given multiplet ($e_g, t_{2g}, \Gamma_8$ etc). For the $e_g$ doublet we are to read off the matrices $\Lambda_j = \langle i | \Lambda_i | j \rangle$ from the transformation equation

$$\Lambda_x |e_g : m\rangle = |e_g : n\rangle M^{d}_{nm},$$

where $|e_g : m\rangle \equiv \{ |d_{x^2-y^2}\rangle, |d_{z^2}\rangle, |d_{x^2-y^2}\rangle, |d_{z}\rangle \}$ is an $e_g$ doublet. Similarly for the $\Gamma_8$ quartet,

$$\Lambda_x |\Gamma_8, \alpha\rangle = |\Gamma_8, \beta\rangle M^{f\alpha}_{\beta\alpha},$$
where the quartet is denoted by $|\Gamma_{\alpha}, \alpha\rangle$, where $\alpha \in [1, 4]$. The result is,

$$
M_{mn}^d = e^{\frac{i\pi x}{2}} \begin{pmatrix}
\frac{i}{2\sqrt{2}} & \frac{i}{2}\sqrt{\frac{1}{2}} & -\frac{i}{2}\sqrt{\frac{1}{2}} & -\frac{i}{2}\sqrt{\frac{1}{2}} \\
-\frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} \\
\frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} \\
-\frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} 
\end{pmatrix},
M_{\alpha\beta}^f = e^{\frac{i\pi x}{2}} \begin{pmatrix}
\frac{1}{2\sqrt{2}} & \sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} \\
-\frac{1}{2\sqrt{2}} & \sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} \\
\frac{1}{2\sqrt{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} \\
-\frac{1}{2\sqrt{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} & -\frac{1}{2}\sqrt{\frac{1}{2}} & \frac{1}{2}\sqrt{\frac{1}{2}} 
\end{pmatrix}.
$$

Note that the rotation cyclically exchanges $x \to y \to z \to x$, thus applying it three times gives overall ”$-1$” due to fermionic statistics.

$$M^3 = -1.$$ 

Finally, we can use (14) to derive the hamiltonian defined in (5) and (6) of the main paper.

**Details of the mean-field theory**

The full Hamiltonian for the problem also contains a term describing the local Hubbard interaction between the $f$-electrons:

$$H_f = U \sum_i \sum_{\alpha=1}^{4} \sum_{\beta \neq \alpha} f_{i\alpha}^\dagger f_{i\alpha} f_{i\beta}^\dagger f_{i\beta}$$

(15)

We consider the infinite $U$, where we can project out all states with occupation number larger than one by replacing the bare $f$-electron fields by Hubbard operators. We represent the Hubbard operators using a slave boson representation, as follows:

$$f_{i\alpha}^\dagger \to X_{\alpha 0}(i) = f_{i\alpha}^\dagger b_i, \quad f_{i\alpha} \to X_{0\alpha}(i) = b_i^\dagger f_{i\alpha},$$

(16)

supplemented by a constraint of no more than one $f$-electron per each site ($U = \infty$):

$$\sum_{\alpha=1}^{4} f_{i\alpha}^\dagger f_{i\alpha} + b_i^\dagger b_i = 1.$$ 

(17)

The partition function corresponding to the model Hamiltonian $H = H_c + H_f + H_{hyb}$ above and with constraint condition (17) reads:

$$Z = \int_{-\pi/\beta}^{\pi/\beta} \frac{\beta d\lambda}{\pi} \int \mathcal{D}(b, b^\dagger, f, f^\dagger, c, c^\dagger) \exp \left( -\int_{0}^{\beta} L(\tau) d\tau \right),$$

(18)

where the Lagrangian $L(\tau)$ is

$$L = \sum_i b_i^\dagger \frac{d}{d\tau} b_i + \sum_{ij} \sum_{\alpha, \beta=1}^{4} f_{i\alpha}^\dagger f_{j\beta}^\dagger \left[ \delta_{ij} \delta_{\alpha\beta} \left( \frac{d}{d\tau} + \varepsilon_f \right) + b_{ij}^\dagger f_{ij, \alpha\beta}^\dagger \right] f_{j\beta} + \sum_{k\sigma} \sum_{a,b=1}^{2} \sum_{c \alpha\kappa} c_{a \kappa}^\dagger \left( \frac{d}{d\tau} + \varepsilon_{ab}(k) \right) c_{b \kappa}$$

$$+ \frac{1}{2} \sum_{k\sigma} \sum_{a=1}^{2} \sum_{\beta=1}^{4} \left( V_{i\alpha, j\beta} c_{a \sigma}^\dagger b_i^\dagger f_{j\beta} + \text{h.c.} \right) + \sum_j i\lambda_j \left( \sum_{\alpha=1}^{4} f_{i\alpha}^\dagger f_{j\alpha} + b_j^\dagger b_j - 1 \right)$$

(19)

Mean-field (saddle-point) approximation corresponds to the following values of the bosonic fields:

$$b_{q}(\tau) = b\delta_{q,0}, \quad i\lambda_{q}(\tau) = (E_f - \varepsilon_f)\delta_{q,0},$$

(20)

where both $a$ and $\varepsilon_f$ are $\tau$-independent. In the mean-field theory we choose a “radial” gauge where the the phase of the $b$-field has been absorbed into the $f$-electron fields. Also, for an insulator, we need a filled quartet of states at each site, so that

$$n_c + n_f = 4.$$ 

(21)
Note, the parameter $b$ also renormalizes the $f$-hopping elements. Indeed, it follows that when $i \neq j$, $f_{i\alpha}^i f_{j\beta} \to X_{\alpha 0}(i) X_{0\beta}(j) = f_{i\alpha}^i b_j b_j f_{j\beta}$. However, the onsite occupancy is unrenormalized by the slave boson fields, since in the infinite $U$ limit, the onsite occupancy $X_{\alpha \alpha}(i) = f_{i\alpha}^i f_{i\alpha}$.

The first three terms together with the last term in the Lagrangian [19] can be written using the new fermionic basis and [20]. It follows:

$$L_0(\tau) = (b^2 - 1)(E_f - \varepsilon_f) + \sum_{\kappa \sigma n=1}^2 \sum_{\kappa n}^2 \xi_{n\kappa}^\dagger \left( \frac{d}{d\tau} + E_{n\kappa}^{(f)} \right) \xi_{n\kappa} + \sum_{\kappa \sigma a=1}^2 \xi_{n\kappa}^\dagger \left( \frac{d}{d\tau} + E_{n\kappa}^{(d)} \right) d_{a\kappa}$$

where the renormalized $f$-electron dispersion is

$$E_{n\kappa}^{(f)} = E_f + 2t_f b^2 \left( c_x + c_y + c_z + (1)^n \sqrt{c_x^2 + c_y^2 + c_z^2 - c_x c_y c_z} \right), \quad n = 1, 2.$$  

Correspondingly, the hybridization matrix in the new fermionic basis can be obtained via unitary transformation with the matrix

$$U_k = \begin{pmatrix} u_k & 0 & v_k & 0 \\ 0 & u_k & 0 & v_k \\ -v_k & 0 & u_k & 0 \\ 0 & -v_k & 0 & u_k \end{pmatrix}, \quad U_k^{-1} = \begin{pmatrix} u_k & 0 & -v_k & 0 \\ 0 & u_k & 0 & -v_k \\ v_k & 0 & u_k & 0 \\ 0 & v_k & 0 & u_k \end{pmatrix}.$$  

Thus we need to calculate the elements of the matrix

$$\tilde{H}_V = iV df \frac{b}{2} \sum_k \xi_{n\kappa}^\dagger H_{hyb}(k) U_k \xi_{n\kappa} + \text{h.c.}$$  

We can use the following relations

$$u_k^2 - v_k^2 = \frac{c_x + c_y - 2c_z}{2R_k}, \quad u_k v_k = \frac{\sqrt{3}}{4R_k} (c_x - c_y).$$  

In our subsequent discussion it will be convenient to write $\tilde{H}_V(k)$ in a more compact form. To derive the corresponding expression we first recall that $H_{hyb}$ can be written as follows

$$H_{hyb}(k) = iV df \frac{b}{2} \left[ \hat{\phi}^z(k) \otimes \hat{\sigma}_x + \hat{\phi}^y(k) \otimes \hat{\sigma}_y + \hat{\phi}^z(k) \otimes \hat{\sigma}_z \right], \quad \hat{\phi}_0 = \hat{\phi}_0^0 \hat{\sigma}_0 + \hat{\phi}_1^0 \hat{\sigma}_z + \hat{\phi}_2^0 \hat{\sigma}_x,$$

$$\tilde{\phi}_0 = \frac{2}{3} (\sin k_x, -\sin k_y, \sin k_z), \quad \tilde{\phi}_1 = \frac{1}{3} (\sin k_x, -\sin k_y, -2 \sin k_z), \quad \tilde{\phi}_2 = \frac{1}{\sqrt{3}} (\sin k_x, \sin k_y, 0).$$

Again, note the change from minus sign to plus sign in front of $\tilde{\phi}_2$ term. This yields the agreement with the hybridization Hamiltonian obtained from the rotations method. We also have

$$\hat{U}_k = u_k \hat{\tau}_0 \otimes \hat{\sigma}_0 + iv_k \hat{\tau}_y \otimes \hat{\sigma}_0, \quad \hat{U}_k^{-1} = u_k \hat{\tau}_0 \otimes \hat{\sigma}_0 - iv_k \hat{\tau}_y \otimes \hat{\sigma}_0,$$

After some algebra we find

$$\hat{U}_k^{-1} \left( \hat{\phi}^x(k) \otimes \hat{\sigma}_x \right) \hat{U}_k = \hat{\tau}_x \otimes \hat{\sigma}_x,$$

$$\hat{U}_k^{-1} \left( \hat{\phi}^y(k) \otimes \hat{\sigma}_y \right) \hat{U}_k = \left( u_k^2 - v_k^2 \right) (\hat{\phi}^y(k) \otimes \hat{\sigma}_y) + 2u_k v_k (\hat{\tau}_x \otimes \hat{\sigma}_y),$$

$$\hat{U}_k^{-1} \left( \hat{\phi}^z(k) \otimes \hat{\sigma}_z \right) \hat{U}_k = \left( u_k^2 - v_k^2 \right) (\hat{\phi}^z(k) \otimes \hat{\sigma}_z) - 2u_k v_k (\hat{\tau}_x \otimes \hat{\sigma}_z).$$

These results become much more transparent if we express $u_k$ and $v_k$ in terms of the angle $\theta_k$:

$$u_k = \cos(\theta_k/2), \quad v_k = \sin(\theta_k/2).$$

Then we see that

$$\hat{U}_k^{-1} \left( \hat{\phi}^z(k) \otimes \hat{\sigma}_x \right) \hat{U}_k = \hat{\phi}^z(k) \otimes \hat{\sigma}_x,$$
where now
\[ \Phi^x = \Phi^x_0 \tau_0 + \Phi^x_1 \tau_z + \Phi^x_2 \tau_x, \quad \Phi^y = \Phi^y_0, \quad \Phi^z = \Phi^z_0 \]
\( \Phi^y_1 = \Phi^y_2 = \Phi^z_1 = \Phi^z_2 = 0 \)
\[ \Phi^x_0 = \phi^x_0, \quad \Phi^y_0 = \phi^y_0, \quad \Phi^z_0 = \phi^z_0. \]

Similarly, we find
\[ \Phi^x = \Phi^x_0 \tau_0 + \Phi^x_1 \tau_z + \Phi^x_2 \tau_x, \quad \Phi^y = \Phi^y_0, \quad \Phi^z = \Phi^z_0 \]
\[ \Phi^y_1 = \Phi^y_2, \quad \Phi^z_1 = \Phi^z_2. \]

Thus, we can re-write (35) as follows
\[ \tilde{H}_V = i V_d \frac{b}{2} \sum_k \delta_{\alpha \beta} \Phi^\alpha \Phi^\beta + h.c., \quad \Phi^\alpha = \Phi^\alpha(x) \otimes \sigma_x + \Phi^\beta(x) \otimes \sigma_y + \Phi^z(x) \otimes \sigma_z \]

Next we derive the mean-field equations.

**Derivation of the mean-field equations**

To derive the mean-field equations we first integrate out \( d \)-electrons by making the following change of variables in the path integral:
\[ d^4 \Phi^d = d^4 \Phi^x \exp \left( \frac{b^2}{4} \Phi^d \Phi^d \right) \]
\[ \tilde{G}_d^{-1}(\omega, \mathbf{k}) = \left[ G_1^{-1}(\omega, \mathbf{k}) \right]^{-1} \]
\[ \tilde{G}_d^{-1}(\omega, \mathbf{k}) = \left[ G_d^{-1}(\omega, \mathbf{k}) \right]^{-1} \]
\[ \tilde{G}_f^{-1}(\omega, \mathbf{k}) = \left[ G_f^{-1}(\omega, \mathbf{k}) \right]^{-1} \]

Then the resulting action is Gaussian and the \( f \)-electrons can be integrated out. This yields the effective action of the form
\[ S_{eff} = (b^2 - 1)(E_f - \varepsilon_f) - T \sum_{\omega} \sum_k \log \det \left[ G_f^{-1}(\omega, \mathbf{k}) \right], \quad \tilde{G}_f^{-1} = \tilde{G}_f^{-1}(\omega, \mathbf{k}) - (V_d \frac{b}{2})^2 \frac{\Phi^d \Phi^d}{\Phi^d \Phi^d} \]

The renormalized \( f \)-electron correlation function \( \tilde{G}_f^{-1} \) has a block diagonal form:
\[ \tilde{G}_f^{-1} = \left( \frac{V_d b^2}{4} \right)^2 \frac{\Phi^d \Phi^d}{\Phi^d \Phi^d} \]

where the diagonal elements are given by
\[ G_1^{-1}(\omega, \mathbf{k}) = \omega - E_{1k} - (V_d \frac{b}{2})^2 \frac{\Phi^d \Phi^d}{\Phi^d \Phi^d} \]
\[ G_2^{-1}(\omega, \mathbf{k}) = \omega - E_{2k} - (V_d \frac{b}{2})^2 \frac{\Phi^d \Phi^d}{\Phi^d \Phi^d} \]
and we have introduced the following functions

\[
\Phi_{1k}^{(\pm)} = (\Phi_0^+ \pm \Phi_1^+)^2 + (\Phi_0^- + \Phi_1^-)^2, \quad \Phi_{2k} = (\Phi_0^+)^2 + (\Phi_0^-)^2,
\]

\[
\Delta_{1k} = \Phi_2^0 (\Phi_0^+ + \Phi_1^+) + (\Phi_2^0 + i\Phi_2^0) [\Phi_0^- + \Phi_1^- - i(\Phi_0^- + \Phi_1^-)],
\]

\[
\Delta_{2k} = \Phi_2^0 (\Phi_0^- - \Phi_1^+) + (\Phi_2^0 - i\Phi_2^0) [\Phi_0^+ - \Phi_1^+ + i(\Phi_0^+ - \Phi_1^+)],
\]

\[
\tilde{\Delta}_{1k} = (\Phi_{1k}^- - i\Phi_{1k}^+)(\Phi_{1k}^+ + \Phi_{1k}^-) - \Phi_{1k}^+ [\Phi_{1k}^- + \Phi_{1k}^- - i(\Phi_{1k}^- + \Phi_{1k}^-)],
\]

\[
\tilde{\Delta}_{2k} = \Phi_{1k}^0 [\Phi_{1k}^- - i(\Phi_{1k}^+ - \Phi_{1k}^-)] - (\Phi_{1k}^- - i\Phi_{1k}^+)(\Phi_{1k}^+ - \Phi_{1k}^-).
\]

Then the determinant of the matrix \( \hat{G}_{ff} \) is

\[
\det \left[ \hat{G}_{ff}^{-1}(i\omega, k) \right] = \left\{ G_{1f}^{-1}(i\omega, k) G_{2f}^{-1}(i\omega, k) - (V_{d} b)^4 \delta_{kk} \right\}^2 \left( \frac{\Delta_{1k}}{i\omega - E_{1k}^{(d)}} + \frac{\Delta_{2k}}{i\omega - E_{2k}^{(d)}} \right) \left( \frac{\tilde{\Delta}_{1k}}{i\omega - E_{1k}^{(d)}} + \frac{\tilde{\Delta}_{2k}}{i\omega - E_{2k}^{(d)}} \right).
\]

Furthermore, we find that

\[
|\Delta_{1k}|^2 + |\tilde{\Delta}_{1k}|^2 = \Phi_{1k}^{(+)}/\Phi_{2k}, \quad |\Delta_{2k}|^2 + |\tilde{\Delta}_{2k}|^2 = \Phi_{1k}^{(-)}/\Phi_{2k}
\]

so that certain terms in the expression \((40)\) will cancel. Therefore, to derive the mean field equation we will need to find the saddle point of the following effective action:

\[
S_{eff} = (b^2 - 1)(E_f - \varepsilon_f) - 2T \sum_{i\omega} \sum_k \log[P_{4k}(i\omega; E_f, b)], \quad P_{4k}(i\omega) = \prod_{i=1}^4 (i\omega - \varepsilon_{ik}).
\]

where we have introduced the polynomial:

\[
P_{4k}(i\omega) = (i\omega - E_{1k}^{(f)})(i\omega - E_{2k}^{(f)})(i\omega - E_{1k}^{(d)})(i\omega - E_{2k}^{(d)}) + (V_{d} b)^4 \delta_{kk} - (V_{d} b)^2 \left\{ [\Phi_{2k}(i\omega - E_{1k}^{(f)}) + \Phi_{1k}^+(i\omega - E_{2k}^{(f)})][i\omega - E_{2k}^{(d)}] + [\Phi_{2k}(i\omega - E_{2k}^{(f)}) + \Phi_{1k}^-(i\omega - E_{1k}^{(f)})][i\omega - E_{1k}^{(d)}] \right\},
\]

\[
\gamma_k^4 = \Phi_{1k}^0 \Phi_{1k}^- + \Phi_{2k}^0 - \Delta_{1k} \Delta_{2k} - \Delta_{1k}^* \Delta_{2k}^* - \Delta_{1k} \Delta_{2k}^* - \Delta_{1k}^* \Delta_{2k}.
\]

Thus, two of the three mean field equations are formally given by

\[
\frac{\partial S_{eff}}{\partial E_f} = 0, \quad \frac{\partial S_{eff}}{\partial b} = 0.
\]

We have

\[
b^2 - 1 + 2 \sum_{i=1}^4 \sum_k f(\varepsilon_{ik}) n_F(\varepsilon_{ik}) = 0, \quad n_F(x) = \frac{1}{e^{\beta x} + 1},
\]

where the function \( f(\varepsilon) \) is:

\[
f(\lambda) = 2\lambda^3 - \lambda^2[2(E_{1k}^{(d)} + E_{2k}^{(d)}) + E_{1k}^{(f)} + E_{2k}^{(f)}] + \lambda(2E_{1k}^{(d)} E_{2k}^{(d)} + (E_{1k}^{(d)} + E_{2k}^{(d)})(E_{1k}^{(f)} + E_{2k}^{(f)}) - (V_{d} b)^2 (\Phi_{1k}^+ + \Phi_{1k}^- + 2\Phi_{2k})]
\]

\[
+ (V_{d} b)^2 [(\Phi_{2k}^- + \Phi_{1k}^+)(E_{1k}^{(d)} + (\Phi_{2k}^- + \Phi_{1k}^+)(E_{2k}^{(d)} - E_{1k}^{(d)} E_{2k}^{(f)} + E_{2k}^{(f)})]
\]

The derivation of the last mean-field equation can be compactly written as follows:

\[
8(E_f - \varepsilon_f) + 2 \sum_{i=1}^4 \sum_k \frac{\partial \varepsilon_{ik}}{\partial E_f} n_F(\varepsilon_{ik}) = 0.
\]