Angle dependent quasiparticle weights in correlated metals

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The main purpose of the present paper is to discuss the variation in the quasiparticle weight $Z$ on moving around the Fermi surface. Indeed $Z$ is a convenient measure of the extent to which Fermi liquid theory works in a Fermi liquid. The theoretical approach we use is the standard hybridization mean field theory for Kondo lattice models of the rare earth alloy. The variation of $Z$ may be linked to the internal orbital structure of the Kondo singlet that forms between the local moments and the conduction electrons. This internal orbital structure derives from the symmetries of the atomic orbital occupied by the local moment and the conduction electron band it is coupled to. In the hybridization mean field theory this leads to angle dependence of the hybridization on going around the Fermi surface. The most dramatic variation occurs when the hybridization vanishes along some directions. Along such hybridization nodes $Z \sim o(1)$ but can become very close to zero along other directions. We demonstrate the possibility of such hybridization nodes in a simplified model appropriate for a Ce-based cubic system. Recent angle resolved photoemission experiments have begun to probe the structure of the electronic excitations of the heavy Fermi liquid. We expect that the physics described in this paper may be probed in the near future.

Inspired by these calculations appropriate to heavy electron systems, we consider the possibility that the pseudogap regime of the underdoped cuprates may actually have a large band-structure Fermi surface but with strongly angle dependent $Z$. Several experimental results on the underdoped cuprates are examined in this light. Such a pseudogap state has some attractive phenomenological features - in particular it provides one possible reconciliation between recent high field quantum oscillation experiments and older ARPES reports of gapless ‘Fermi arcs’. However such a large Fermi surface Fermi liquid state also has a number of problems with other experiments making it unappealing as a serious theory.

I. INTRODUCTION

The normal state of the cuprate materials is often described (at least empirically) as a non-fermi liquid metal. A remarkable feature of this metal is the presence of significant momentum space anisotropy, the extent to which Fermi liquid theory fails depends strikingly on which part of a nominal Fermi surface is being probed. In optimally doped systems the quasiparticle-like peaks measured in photoemission experiments are typically much broader along the ‘antinodal’ direction near the edges of the Brillouin zone than along the diagonal ‘nodal’ direction. The difference is even more striking in the underdoped cuprates where a pseudogap opens - apparently only near the antinodal regions leaving behind a gapless ‘Fermi arc’ centered at four nodal points. Somewhat similar phenomena have been reported even in the overdoped cuprates based on transport experiments though the anisotropy weakens with increasing doping.

Theoretical understanding of such phenomena in the cuprates is primitive and is hampered by the lack of a suitable framework for describing non-fermi liquid phenomena. However the cuprates are but one example of a host of correlated metals that have been studied over the years. Fermi liquid theory does not always fail in such metals. Motivated by the observed momentum space anisotropy in the cuprates we therefore pose the opposite general question: does the extent to which Fermi liquid theory work depend dramatically on where one is on the Fermi surface in a correlated Fermi liquid metal? As there is a firm theoretical framework to discuss Fermi liquid metals, this question can be expected to yield more easily to progress.

The most celebrated success of Fermi liquid theory is provided by the ‘heavy Fermi liquid’ state of rare earth alloys. These have quasiparticle effective masses as high as 100-1000 times the bare electron mass and an associated small quasiparticle weight $Z$ at the Fermi surface. The extent to which Fermi liquid theory works in the cuprates we therefore pose the open question: does the extent to which Fermi liquid theory fails in such metals. Motivated by the observed momentum space anisotropy in the cuprates we therefore pose the opposite general question: does the extent to which Fermi liquid theory work depend dramatically on where one is on the Fermi surface in a correlated Fermi liquid metal? As there is a firm theoretical framework to discuss Fermi liquid metals, this question can be expected to yield more easily to progress.

The most celebrated success of Fermi liquid theory is provided by the ‘heavy Fermi liquid’ state of rare earth alloys. These have quasiparticle effective masses as high as 100-1000 times the bare electron mass and an associated small quasiparticle weight $Z$ at the Fermi surface. The main purpose of the present paper is to discuss the variation in the quasiparticle weight $Z$ on moving around the Fermi surface. Indeed $Z$ is a convenient measure of the extent to which Fermi liquid theory works in a Fermi liquid. The theoretical approach we use is the standard hybridization mean field theory for Kondo lattice models of the rare earth alloy. The variation of $Z$ may be linked to the internal orbital structure of the Kondo singlet that forms between the local moments and the conduction electrons. This internal orbital structure derives from the symmetries of the atomic orbital occupied by the local moment and the conduction electron band it is coupled to. In the hybridization mean field theory this leads to angle dependence of the hybridization on going around the Fermi surface. The most dramatic variation occurs when the hybridization vanishes along some directions. Along such hybridization nodes $Z \sim o(1)$ but can become very close to zero along other directions. We demonstrate the possibility of such hybridization nodes in a simplified model appropriate for a Ce-based cubic system. Recent angle resolved photoemission experiments have begun to probe the structure of the electronic excitations of the heavy Fermi liquid. We expect that the physics described in this paper may be probed in the near future.

Inspired by these calculations appropriate to heavy electron systems, we consider the possibility that the pseudogap regime of the underdoped cuprates may actually have a large band-structure Fermi surface but with strongly angle dependent $Z$. Several experimental results on the underdoped cuprates are examined in this light. Such a pseudogap state has some attractive phenomenological features - in particular it provides one possible reconciliation between recent high field quantum oscillation experiments and older ARPES reports of gapless ‘Fermi arcs’. However such a large Fermi surface Fermi liquid state also has a number of problems with other experiments making it unappealing as a serious theory.
of the underdoped cuprates. A non-fermi liquid version of such a large Fermi surface state might perhaps resolve these difficulties but theoretical description of such a state remains out of reach.

II. KONDO SINGLETS WITH INTERNAL ORBITAL STRUCTURE

The heavy fermion materials are conveniently modeled as Kondo lattices, i.e. a periodic lattice of local moments coupled by magnetic exchange to a separate band of conduction electrons. At low temperatures the local moments are absorbed into the Fermi sea of the metal through Kondo singlet formation. In a typical heavy electron metal the local moments occupy atomic $f$-orbitals. The conduction electrons derive from bands with different symmetry ($s$, $p$ or $d$). The Kondo singlet that forms between a local moment and a conduction electron will therefore have nontrivial internal orbital structure. In the low temperature heavy fermi liquid phase this orbital structure leads to pronounced anisotropies between various parts of the Fermi surface. A close analogy is with the physics of unconventional superconductors where Cooper pairs with non-trivial internal orbital structure condense leading to anisotropic superconductivity. In the heavy Fermi liquid case such anisotropic effective masses are known to occur and have been discussed theoretically using a renormalized band theory approach.

In the present paper we will mainly focus on the quasiparticle spectral weight $Z$ which is a measure of the extent to which Fermi liquid theory works. To illustrate our point we focus specifically on Ce based heavy electron materials with the Ce ion in a $f^1$ state. We also assume cubic symmetry. Such a Ce ion has, after considering the effect of spin-orbit coupling and crystal field splitting, a low energy Kramers doublet that couples to a separate conduction band. We treat the corresponding Kondo lattice model within the slave boson mean field approach. This approach is particularly well suited to describing the heavy Fermi liquid phase. At the mean field level there are two bands - one derived from the f-moments and the other from the conduction electrons - that are hybridized. Physically the hybridization amplitude is a measure of the Kondo singlet formation. We show that this amplitude has strong momentum dependence coming from the symmetry of the f-orbital. Thus the true quasiparticles at the fermi surface are angle dependent admixtures of the $f$-fermions and the conduction electrons. Most remarkably we show that our simplified model naturally has directions where the hybridization vanishes. These hybridization nodes have a number of consequences. Most importantly it leads to a fermi surface structure where along the hybridization nodes the true (large) Fermi surface is contained within the original small Fermi surface of the conduction electrons. Thus along these directions the true quasiparticle mostly has $c$-character with weak admixture to $f$. Along other directions the situation is reversed. Now the physical electron spectral weight depends on the extent to which the conduction electron contributes to the quasiparticle state of the true large Fermi surface. This then leads to the dramatic variation of the quasiparticle weight discussed in the Introduction.

In passing we note that hybridization nodes have previously been proposed in the context of theories of gapless Kondo insulators. When present such nodes have rather different effects in metallic heavy electron systems as we discuss below. Hybridization nodes are also present in toy Kondo lattice models where each local moment is coupled to a conduction electron at a neighboring site. Though such models are not directly relevant to heavy electron systems they capture some of the same physics described in this paper.

III. ANDERSON MODEL FOR A CERIUM ION

We begin by briefly reviewing the Anderson model describing a Cerium $f^1$ impurity in a metallic host. The $f$ states have orbital angular momentum $l = 3$ so that on including the spin there are $2 \times (3 + 1) = 14$ quantum states in this orbital. Spin-orbit coupling breaks the degeneracy of this orbital into two sets of states with $J = 7/2$ and $J = 5/2$ where $J$ is the total angular momentum ($J = s + l$). The $J = 5/2$ states have lower energy and so we will concentrate on them. In a cubic environment crystal fields will further split the $J = 5/2$ states into a doublet (lower energy) and a quadruplet (higher energy) states. We will concentrate on the lower energy doublet described by $|M = 1 > = (\frac{1}{6})^{1/2} |J_z = \frac{5}{2} > - (\frac{5}{6})^{1/2} |J_z = \frac{3}{2} >$,

$|M = 2 > = (\frac{1}{6})^{1/2} |J_z = \frac{5}{2} > - (\frac{5}{6})^{1/2} |J_z = -\frac{3}{2} >$.

As expected these states go into each other under time reversal. Now consider coupling of this doublet to a band of conduction electrons $c_{k\sigma}$. We assume that the $f$-electron in a state $M$ can hybridize with the appropriate partial wave of the $c$-electron also in the same state $M$. The coupling may therefore be modeled by the Anderson impurity Hamiltonian.

$$H = \sum_{k,M} \varepsilon_k c_{k,M}^{\dagger} c_k + \mu_f \sum_M f_M^{\dagger} f_M + U \sum_{M,M'} n_{M} n_{M'},$$

$$+ \sum_{k,M} V_k c_{k,M}^{\dagger} f_M + V_k^{\dagger} f_M^{\dagger} c_{k,M},$$

(2)

with the electron partial wave operator $c_{k,M}$ defined through

$$c_{k,M}^{\dagger} = \frac{1}{2\pi} \int \frac{d\Omega^k}{4\pi} c_{k,M}^{\dagger}(k,\sigma|k,M),$$

(3)
where the integral is taken over all directions of the vector \( \mathbf{k} \). For simplicity we assume further that \( V_k = V \) independent of \( k \).

Focussing now on the strong correlation limit of large \( U \) we restrict the \( f \)-occupation to be one, i.e. we impose the constraint

\[
\sum_M f_M^\dagger f_M = 1. \tag{4}
\]

The standard Schrieffer-Wolf transformation\cite{18,19} then gives the “Kondo” effective Hamiltonian with an interaction

\[
H_I = J \sum_{k,k',M,M'} f_M^\dagger c_{k,M} c_{k',M'} f_{M'} \tag{5}
\]

with \( J = V^2 U / [\mu_f (\mu_f + U)] \). This is a Kondo type\cite{20} interaction and describes the coupling of the fluctuating \( M \) state at the \( Ce \) site to the conduction band. Alternately we may write

\[
H_I = J \sum_{k,k',\sigma,\sigma',M,M'} \langle k',\sigma' | k'M' > < kM | \sigma > f_M^\dagger c_{\sigma'} c_{\sigma' \dagger} f_{M'}, \tag{6}
\]

so that we may write

\[
H_I = J \sum_{\mathbf{R},k,k',\sigma,\sigma',M,M'} \langle \mathbf{k}',\sigma' | \mathbf{k}' M' > < \mathbf{k} M | \sigma > f_{\mathbf{R},M}^\dagger c_{\sigma'} c_{\sigma' \dagger} f_{\mathbf{R}, M'}. \tag{7}
\]

where \( |k,M,R\rangle \) is a \( c \)-electron partial wave centered at site \( \mathbf{R} \). We have

\[
|k,M,R\rangle = e^{i \mathbf{P} \cdot \mathbf{R}} |k,M\rangle, \tag{8}
\]

where \( \mathbf{P} \) is the momentum operator (generator of translation) and \( |k,M\rangle \) is a partial wave centered at the origin. Thus we get:

\[
\langle \mathbf{k},\sigma | k,M,R \rangle = \langle \mathbf{k},\sigma | e^{i \mathbf{P} \cdot \mathbf{R}} |k,M\rangle = e^{i \mathbf{k} \cdot \mathbf{R}} \langle \mathbf{k},\sigma | k,M \rangle, \tag{9}
\]

since \( (\mathbf{k},\sigma) \) is momentum eigenstate. With Fourier transforming the \( c_{\mathbf{k}\sigma} \) electrons back to real space \( (c_{\mathbf{k}\sigma} = \sum_{\mathbf{R}} e^{i \mathbf{k} \cdot \mathbf{R}} c_{\mathbf{R}\sigma}) \) we get:

\[
H_K = J \sum_{\mathbf{R},\mathbf{R}',M,M'} \sum_{\mathbf{k}\sigma} f_{\mathbf{R},M}^\dagger \left[ \sum_{\mathbf{k}\sigma} \langle k,M | k,M \rangle e^{i \mathbf{k} \cdot (\mathbf{R} - \mathbf{R})} c_{\mathbf{R}\sigma} \right]
\]

\[
\times \left[ \sum_{\mathbf{k}',\sigma'} \langle \mathbf{k}',\sigma' | \mathbf{k}',M' \rangle e^{-i \mathbf{k}' \cdot (\mathbf{R'} - \mathbf{R})} c_{\mathbf{R}\sigma}' \dagger \right] f_{\mathbf{R}',M'} \tag{10}
\]

IV. KONDO LATTICE MODEL

We now generalize the description of a single \( Ce \) impurity ion of the previous section to a lattice of \( Ce \) ions. We first introduce operators \( f_{\mathbf{R},M} \) for the local moments at site \( \mathbf{R} \) of the lattice. The generalization of the Kondo interaction \( H_I \) is clearly

\[
H_K = J \sum_{\mathbf{R},\mathbf{R}',M,M'} \sum_{\mathbf{k}\sigma} \langle \mathbf{k}',\sigma' | \mathbf{k}',M' \rangle \langle \mathbf{k},M,\mathbf{R} | \mathbf{k},\sigma \rangle f_{\mathbf{R},M}^\dagger c_{\sigma'} c_{\sigma' \dagger} f_{\mathbf{R}',M'}. \tag{11}
\]

It is convenient now to define real space operators

\[
\Gamma_{\mathbf{R},\mathbf{R}',M} = \sum_{\mathbf{k},\sigma} \langle k,M | \mathbf{k},\sigma \rangle e^{i \mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} c_{\mathbf{R}\sigma}, \tag{12}
\]

which are a mixture of spin up and down electrons. In terms of these real-space operators, the Kondo interaction assumes simple form:

\[
H_K = J \sum_{\mathbf{R},\mathbf{R}',M,M'} \sum_{\mathbf{k},\sigma} f_{\mathbf{R},M}^\dagger f_{\mathbf{R}',M'} \Gamma_{\mathbf{R},\mathbf{R}',M} \Gamma_{\mathbf{R}',\mathbf{R},M'}^\dagger f_{\mathbf{R},M'} f_{\mathbf{R}',M'} - \mu_f \langle \sum_{\mathbf{R}M} f_{\mathbf{R},M}^\dagger f_{\mathbf{R},M} \rangle \tag{13}
\]

The full Kondo lattice model then takes the form

\[
H = H_c + H_K \tag{14}
\]

together with the constraints

\[
\sum_{\mathbf{M}} f_{\mathbf{M},\mathbf{R}}^\dagger f_{\mathbf{M},\mathbf{R}} = 1, \tag{15}
\]

at each site \( \mathbf{R} \). Note that due to this constraint it is no longer appropriate to think of the \( f \)-operators as describing physical electrons. Rather at this stage they should be viewed as neutral fermions that carry spin alone. As is well known this representation is redundant and introduces an extra \( U(1) \) gauge structure associated with the freedom to change the phase of \( f \) independently at each site.

V. SLAVE BOSON MEAN FIELD THEORY

We now discuss the Fermi liquid phases described by this Kondo lattice model within the slave boson mean field approximation. In simpler Kondo lattice models this technique correctly captures the essential physics of the fermi liquid state.\cite{21} In the mean field we impose the constraint of Eqn. (15) on average with a chemical potential \( \mu_f \) for the \( f \)-fermions and replace the Kondo interaction by a self-consistently determined hybridization between the \( c \) and \( f \) operators. The mean field Hamiltonian reads

\[
H_{MF} = \sum_{\mathbf{R}\mathbf{M}} \varepsilon_{\mathbf{kM}} c_{\mathbf{kM}}^\dagger c_{\mathbf{kM}} + \mu_f \sum_{\mathbf{R}\mathbf{M}} f_{\mathbf{R}\mathbf{M}}^\dagger f_{\mathbf{R}\mathbf{M}}
\]

\[
+ b \sum_{\mathbf{R}\mathbf{M}} \left( f_{\mathbf{R}\mathbf{M}}^\dagger \sum_{\mathbf{R}M} \Gamma_{\mathbf{R}M} + h.c. \right) \tag{16}
\]

The mean field parameters \( \mu_f \), \( b \) must be determined self-consistently through the equations

\[
1 = \sum_{\mathbf{M}} \langle f_{\mathbf{M},\mathbf{R}}^\dagger f_{\mathbf{M},\mathbf{R}} \rangle, \tag{17}
\]

\[
b = \sum_{\mathbf{M}} \langle f_{\mathbf{M},\mathbf{R}}^\dagger f_{\mathbf{M},\mathbf{R}} \sum_{\mathbf{R}M} \Gamma_{\mathbf{R}M} \rangle. \tag{18}
\]
Note that we have chosen $b$ to be real in this mean field. Parenthetically we note that a non-zero mean field hybridization parameter $b$ should really be viewed as a Higgs condensate for the $U(1)$ gauge structure introduced when we represent the spins in terms of the $f$-fields. In this Higgs phase the internal gauge charge of the $f$-fermions is screened by the condensate and the resulting screened gauge neutral object has the same quantum numbers as the electron. This structure of the low energy electrons manifests itself as a small electron quasiparticle weight at the heavy electron Fermi surface.

To diagonalize this mean field Hamiltonian we go to momentum space. We write $f_{M,R} = \sum_q e^{-i\mathbf{q}\cdot\mathbf{R}} f_{M,q}$ and put in original form of $\Gamma$ operators in terms of $c$. The hybridization term then becomes

$$H_{MF} = b \sum_{\mathbf{R},\mathbf{r}, q} \sum_\mathbf{q,k,\sigma} \langle k, M | \mathbf{k}, \sigma \rangle e^{i\mathbf{k} \cdot \mathbf{R}} c_{\mathbf{r},\sigma} + \text{h.c.}$$

$$= b \sum_{\mathbf{q}, \mathbf{k}, \sigma, r} \left( \sum_{\mathbf{R}} e^{i\mathbf{q} \cdot \mathbf{k} - \mathbf{R}} f_{M,\mathbf{q}} \langle k, M | \mathbf{k}, \sigma \rangle \right) \times \left( \sum_{\mathbf{r}} e^{i\mathbf{r} \cdot \mathbf{c}_{\mathbf{r},\sigma}} \right) + \text{h.c.}$$

$$= b \sum_{\mathbf{k}} \langle k, M | \mathbf{k}, \sigma \rangle f_{M,\mathbf{k}} c_{\mathbf{k},\sigma} + \text{h.c.}. \quad (19)$$

Thus the momentum dependence of the hybridization is captured through the $\langle k, \sigma | k, M \rangle$ matrix element, which we calculate in the Appendix.

We define the four component field $\Psi_{\mathbf{k}}$

$$\Psi_{\mathbf{k}} = \begin{bmatrix} c_{\mathbf{k}1} \\ c_{\mathbf{k}2} \\ f_{\mathbf{k}1,1} \\ f_{\mathbf{k}2,2} \end{bmatrix},$$

in terms of which, the Hamiltonian becomes

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \begin{bmatrix} \varepsilon_{\mathbf{k}} \mathbb{I} & b M(\mathbf{k}) \\ b M^\dagger(\mathbf{k}) & \mu_f \mathbb{I} \end{bmatrix} \Psi_{\mathbf{k}}. \quad (20)$$

Here $M(\mathbf{k})$ is a $2 \times 2$ matrix given by

$$M(\mathbf{k}) = \begin{bmatrix} B(\mathbf{k}) & A^*(\mathbf{k}) \\ A(\mathbf{k}) & -B^*(\mathbf{k}) \end{bmatrix}. \quad (21)$$

The functions $A(\mathbf{k}), B(\mathbf{k})$ are defined in the Appendix.

Now we look for operators $\gamma_i(\mathbf{k})$ that satisfy $[H_{MF}, \gamma_i(\mathbf{k})] = \lambda_i(\mathbf{k}) \gamma_i(\mathbf{k})$, in term of which $H_{MF}$ is diagonal:

$$H_{MF} = \sum_{i,k} \lambda_i(\mathbf{k}) \gamma_i(\mathbf{k})^\dagger \gamma_i(\mathbf{k}). \quad (22)$$

If we express $\gamma_i(\mathbf{k})$ as:

$$\gamma_i(\mathbf{k}) = u_i^1(\mathbf{k}) c_{\mathbf{k}1} + u_i^2(\mathbf{k}) c_{\mathbf{k}2} + u_i^3(\mathbf{k}) f_{\mathbf{k}1,1} + u_i^4(\mathbf{k}) f_{\mathbf{k}2,2}, \quad (23)$$

where the coefficients $u_i^\sigma(\mathbf{k})$ are determined through the eigenvalue equation:

$$\begin{bmatrix} \varepsilon_{\mathbf{k}} \mathbb{I} & b M(\mathbf{k}) \\ b M^\dagger(\mathbf{k}) & \mu_f \mathbb{I} \end{bmatrix} \begin{bmatrix} u_1^1(\mathbf{k}) \\ u_1^2(\mathbf{k}) \\ u_1^3(\mathbf{k}) \\ u_1^4(\mathbf{k}) \end{bmatrix} = \lambda_i(\mathbf{k}) \begin{bmatrix} u_1^1(\mathbf{k}) \\ u_1^2(\mathbf{k}) \\ u_1^3(\mathbf{k}) \\ u_1^4(\mathbf{k}) \end{bmatrix} \quad (24)$$

From this we get the four eigenstates and the corresponding dispersion of four bands:

$$\lambda_1(\mathbf{k}) = \frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} - \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \mu_f}{2}\right)^2 + b^2(|A(\mathbf{k})|^2 + |B(\mathbf{k})|^2)},$$

$$\lambda_2(\mathbf{k}) = \frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} - \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \mu_f}{2}\right)^2 + b^2(|A(\mathbf{k})|^2 + |B(\mathbf{k})|^2)},$$

$$\lambda_3(\mathbf{k}) = \frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} + \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \mu_f}{2}\right)^2 + b^2(|A(\mathbf{k})|^2 + |B(\mathbf{k})|^2)},$$

$$\lambda_4(\mathbf{k}) = \frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} + \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \mu_f}{2}\right)^2 + b^2(|A(\mathbf{k})|^2 + |B(\mathbf{k})|^2)}.$$

At each $\mathbf{k}$ obviously we have $\lambda_1(\mathbf{k}) = \lambda_2(\mathbf{k}) \leq \lambda_3(\mathbf{k}) = \lambda_4(\mathbf{k})$, so we have two sets of doubly-degenerate bands. The degeneracy is a consequence of time reversal and inversion symmetries which have been assumed in the original model.

Let us assume that there are $n_c$ conduction electrons per unit cell with $n_c < 1$. Once combined with single $f$-fermion per unit cell, we then need to fill these bands up to the Fermi energy to give a total particle number of $1 + n_c$ per unit cell. Only one states in the lower bands $\lambda_1$ and $\lambda_2$ are $e$ filled, and the Fermi surface always lives in these two bands. Clearly the Fermi surface is large in that its volume counts both the conduction electrons and the $f$-fermions. The shape of the Fermi surface corresponding to our simple model is shown shown in Fig. [1].

We note that the hybridization matrix $b M(\mathbf{k})$ vanishes along the (100) and symmetry related directions (see Appendix). These hybridization nodes lead to striking Fermi surface anisotropies as discussed in detail below. For now we note that along these ‘nodal’ directions the Fermi surface coincides with the original small conduction electron Fermi surface. To see this consider the spectrum of the partially occupied band. It is obvious that $\lambda(\mathbf{k}) < \frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} - \frac{|\varepsilon_{\mathbf{k}} - \mu_f|}{2}$. On the other hand $\frac{\varepsilon_{\mathbf{k}} + \mu_f}{2} - \frac{|\varepsilon_{\mathbf{k}} - \mu_f|}{2} = \min(\varepsilon_{\mathbf{k}}, \mu_f)$ so that for all $\mathbf{k}, \lambda(\mathbf{k}) \leq \mu_f$ (equality only holds for the points where
where for simplicity we have assumed that the energy to add, or remove an $f$-electron is $U$. Here $\ket{n}$ denote the first excited states. To a good approximation, the state-vector in the second term is given by written as $\left(f_M^\dagger \psi_{\kappa,\sigma} + c_{\kappa,\sigma}^\dagger f_M\right)\ket{g_0}$. Now when we annihilate an electron by acting with $\psi$ on $\ket{g_1}$ state, only final states which lie within the manifold of states with single $f$-occupation at the impurity, site will contribute to the photoemission intensity at low energy. There are two such states, one corresponding to the action of $c$ on the $\bra{g_0}f$ component of the ground state, and the other corresponding to the action of $f$ on the second term in $\bra{g_1}$ (i.e. on the $f^\dagger c\ket{g_0}$ term). The net action of $\psi_{\kappa,\sigma}$ on $\ket{g_0}$ is then:

$$\psi_{\kappa,\sigma} \sim \psi_{\kappa,\sigma} + (V/U) \sum_{\kappa',\sigma',M',M} \bra{k',M'|k',\sigma'} \times \bra{k,\sigma|k,M}f_M^\dagger c_{\kappa',\sigma'} f_M.$$

The first term corresponds to the knocking off an electron from the $c$ band and second term corresponds to the first order process where an electron from an $f$ orbital is knocked off and an electron from $c$ band replaces it. Now for a lattice of impurities, we should consider processes where $f$ electrons from different sites are knocked out:

$$\psi_{\kappa,\sigma} \sim \psi_{\kappa,\sigma} + (V/U) \sum_{\kappa',\sigma',M',M} \sum_{\mathbf{R}} \bra{k',M',\mathbf{R}|k',\sigma'} \times \bra{k,\sigma|k,M,\mathbf{R}}f_M^\dagger c_{\kappa',\sigma'} f_M.$$

It is convenient to reexpress this in real space. The
procedure is the same we did in section \[ V \]

\[
\sum_{\mathbf{R}} \sum_{\mathbf{k}', \mathbf{\sigma}', \mathbf{\sigma}''} \langle k', M', \mathbf{R} | \mathbf{k}', \mathbf{\sigma}' \rangle \langle k, \mathbf{\sigma} | k, M, \mathbf{R} \rangle f_{M', \mathbf{R}}^{\mathbf{k}', \mathbf{\sigma}'} f_{M, \mathbf{R}}^{\mathbf{k}, \mathbf{\sigma}''} = \sum_{\mathbf{R}} \sum_{\mathbf{k}', \mathbf{\sigma}', \mathbf{\sigma}''} \langle k', M' | k', \mathbf{\sigma}' \rangle e^{i \mathbf{k}' \cdot (\mathbf{r} - \mathbf{R})} f_{M', \mathbf{R}}^{k', \mathbf{\sigma}'}
\]

\[= \sum_{\mathbf{R}} \sum_{M} f_{M', \mathbf{R}}^{\mathbf{k}', \mathbf{\sigma}'} \left[ \langle k', M' | k', \mathbf{\sigma}' \rangle e^{i \mathbf{k}' \cdot (\mathbf{r} - \mathbf{R})} \mathbf{c}_{k', \mathbf{\sigma}'} \right] \sum_{\mathbf{R}} e^{i \mathbf{k} \cdot \mathbf{R}} f_{M, \mathbf{R}}
\]

\[= \sum_{\mathbf{R}} \sum_{M} f_{M', \mathbf{R}}^{\mathbf{k}', \mathbf{\sigma}'} \mathbf{c}_{k', \mathbf{\sigma}'} \sum_{\mathbf{M}} \langle k, \mathbf{\sigma} | k, M, \mathbf{R} \rangle f_{M, \mathbf{R}}
\]

\[= \sum_{\mathbf{R}} \sum_{M} f_{M', \mathbf{R}}^{\mathbf{k}', \mathbf{\sigma}'} \mathbf{c}_{k', \mathbf{\sigma}'} \sum_{\mathbf{M}} \langle k, \mathbf{\sigma} | k, M, \mathbf{R} \rangle f_{M, \mathbf{R}}.
\]

(29)

Within the slave boson mean field approximation we replace the product \( f^c c \) (or equivalently \( f^\dagger \Gamma \)) term in the second term by its average to get:

\[\psi_{k, \mathbf{\sigma}} \sim c_{k, \mathbf{\sigma}} + (b/V) \sum_{\mathbf{M}} \langle k, \mathbf{\sigma} | k, M, \mathbf{R} \rangle f_{M, \mathbf{R}}.
\]

(30)

The ARPES intensity may now be calculated from the Greens function of this \( \psi \) operator. Its trace is given by

\[Tr \left[ G_{\mathbf{\sigma} \mathbf{\sigma}'}(k, i \omega_n) \right] = \int_0^{\beta} d\tau e^{i \omega_n \tau}
\]

\[\langle T_\tau \left[ \psi_1 k, \tau \psi_1^\dagger k, 0 \right] \psi_1 k, \tau \psi_1^\dagger k, 0 \rangle \right]
\]

where the expectation value is taken in the ground state. From equation (30) it is obvious that this green function consists of four different terms. For this calculation, we need to have \( c_{\mathbf{\sigma}} \) and \( f_{M} \) operators, in term of \( \gamma \) operators. To make this calculation more transparent, it is useful to introduce the unitary matrix \( U \) as:

\[U = \begin{bmatrix}
  u_1^1 & u_1^2 & u_1^3 & u_1^4 \\
  u_2^1 & u_2^2 & u_2^3 & u_2^4 \\
  u_3^1 & u_3^2 & u_3^3 & u_3^4 \\
  u_4^1 & u_4^2 & u_4^3 & u_4^4
\end{bmatrix}
\]

(32)

where:

\[\begin{bmatrix}
  \gamma_1^1 \\
  \gamma_2^1 \\
  \gamma_3^1 \\
  \gamma_4^1
\end{bmatrix} = U \begin{bmatrix}
  c_1^1 \\
  c_1^2 \\
  c_1^3 \\
  c_1^4
\end{bmatrix}.
\]

(33)

Here \( \mathbf{k} \) index is suppressed for notational convenience. Inverting we get

\[c_1^1 = u_1^1 \gamma_1^1 + u_2^1 \gamma_2^1 + u_3^1 \gamma_3^1 + u_4^1 \gamma_4^1,
\]

(34)

\[c_1^2 = u_1^2 \gamma_1^1 + u_2^2 \gamma_2^1 + u_3^2 \gamma_3^1 + u_4^2 \gamma_4^1,
\]

(35)

\[f_1^1 = u_1^1 \gamma_1^1 + u_2^1 \gamma_2^1 + u_3^1 \gamma_3^1 + u_4^1 \gamma_4^1,
\]

(36)

\[f_1^2 = u_1^2 \gamma_1^1 + u_2^2 \gamma_2^1 + u_3^2 \gamma_3^1 + u_4^2 \gamma_4^1.
\]

(37)

Using this result, we can expand imaginary part of the trace of the Green function to obtain the zero temperature spectral function. This has four terms corresponding to the operator combinations \( cc^\dagger, f f^\dagger, cc^\dagger \) and \( cc^\dagger \). Let us calculate them one by one. The \( cc^\dagger \) term is:

\[Z_{cc}(k, \omega) = (|u_1^1(k)|^2 + |u_1^2(k)|^2) \delta(\lambda_1(k) - \omega)\]

\[+ (|u_2^1(k)|^2 + |u_2^2(k)|^2) \delta(\lambda_2(k) - \omega).
\]

(38)

We then get the following form for the quasi-particle residue on the fermi surface:

\[Z_{cc}(k, \lambda_2(k) = E_f) = |u_1^1(k)|^2 + |u_1^2(k)|^2 = \frac{b(k)^2}{b(k)^2 + \left( \frac{\epsilon(k) - \mu_f}{2} + \sqrt{\left( \frac{\epsilon(k) - \mu_f}{2} \right)^2 + b(k)^2} \right)^2}
\]

(39)

Now for \( f f^\dagger \) term (noting \( u_1^1 = u_2^1 = 0 \)) we have:

\[A_{ff}(k, \omega) = \frac{(b(k)^2)}{V} \left[ |u_1^3(k)|^2 \delta(\lambda_1(k) - \omega)\right.\]

\[+ \left. \left( \frac{b(k)^2}{V} \right)^2 |u_2^3(k)|^2 \delta(\lambda_2(k) - \omega). \right]
\]

(40)

This gives the residue:

\[Z_{ff}(k, \lambda_2(k) = E_f) = \frac{\left( \frac{\epsilon(k) - \mu_f}{2} + \sqrt{\left( \frac{\epsilon(k) - \mu_f}{2} \right)^2 + b(k)^2} \right)^2}{b(k)^2 + \left( \frac{\epsilon(k) - \mu_f}{2} + \sqrt{\left( \frac{\epsilon(k) - \mu_f}{2} \right)^2 + b(k)^2} \right)^2}
\]

(41)

The last contribution will be:

\[Z_{cf}(k, \lambda_2(k) = E_f) = \frac{2(b^2/V)}{\left( \frac{\epsilon(k) - \mu_f}{2} + \sqrt{\left( \frac{\epsilon(k) - \mu_f}{2} \right)^2 + b(k)^2} \right)^2}
\]

\[\times \text{Re} \left( A^2(\Omega_k) + B^2(\Omega_k) \right).
\]

(42)

where \( b(k) = b \sqrt{|A(\Omega_k)|^2 + |B(\Omega_k)|^2} \). In Fig. [1] we have also indicated the total residue \( Z_{total} \) which is the sum of these three contributions.

Using the fact that \( |b(k)| \) is small, we can investigate the behavior of \( Z_{total} \) at least for the points where \( |b(k)| \ll |\epsilon(k) - \mu_f| \). For such points we see that whenever \( c_k > \mu_f \) the dominant term (of order \( b^2/V^2 \)) is \( Z_{ff} \) and it varies since \( b(k) \) is angle dependent. On the other hand, when \( c_k < \mu_f \), the dominant contribution is \( Z_{cc} \) which is of order one. This information could be summarized in the following form:

\[Z(k, \lambda_2(k) = E_f) = \frac{b^2}{\left( \frac{\epsilon(k) - \mu_f}{2} \right)^2} \theta(\epsilon(k) - \mu_f) + \theta(\mu_f - \epsilon(k)).
\]

(43)
A key result of this calculation is that for the points where \( \varepsilon(k) > \mu_f \), \( Z \) is small and of order \( \frac{b(k)^2}{(\varepsilon(k) - \mu_f)^2} \); this quantity has varies by about 20% due to the angle dependent \( b(k) \). But for the points where \( \mu_f > \varepsilon(k) \), the quasi-particle residue will be of order one and will exhibit no strong variations. The small region in the middle of Fermi surface in Fig. [1] with \( Z \sim 1 \) corresponds is these points. These regions are centered along \( (100) \) and symmetry related directions. As discussed in the previous section the hybridization matrix has nodes in these special directions and the corresponding quasiparticles are essentially conduction electrons with \( Z \sim 1 \). On the other hand further away from these nodal directions the quasiparticles develop \( f \)-character and \( Z \sim o(b^2) \) along these other directions.

There is thus a dramatic anisotropy in \( Z \) on moving around the Fermi surface. We note that ARPES experiments will naturally be able to resolve the quasiparticle peak along high-\( Z \) directions. However a low resolution ARPES study may well not be able to resolve the small-\( Z \) quasiparticles at all and may incorrectly conclude that the fermi surface consists only of finite open ended pieces.

VII. MOMENTUM DEPENDENT EFFECTIVE MASS

It is well known that the effective mass \( m^* \) in a heavy fermion system can be very anisotropic on the Fermi surface. How do these anisotropies correlate with the anisotropic \( Z \)? It is precisely the combination \( Z \times m^* \) that determines the tunneling density of states. It is therefore also interesting to look at \( m^*(k) \) variations over the Fermi surface. The effective mass can be calculated by taking the second derivative of energy with respect to momentum in direction perpendicular to the Fermi surface i.e. \( \frac{\partial^2 \varepsilon(k)}{\partial k_z^2} \):

\[
\frac{1}{m^*(k)} = \frac{1}{2m^*_{e}} \left[ 1 - \frac{\varepsilon_k - \mu_f}{2} \sqrt{\frac{\varepsilon_k - \mu_f}{2} + b(k)^2} + \frac{b^2(\varepsilon_k - \mu_f)f(k)}{\left(\frac{\varepsilon_k - \mu_f}{2} + b(k)^2\right)^{3/2}} \right]
\approx \frac{1}{m^*_{e}} \left[ \Theta(\mu_f - \varepsilon(k)) + \frac{b^2}{(\varepsilon_k - \mu_f)^2}g(k) \right]
\]

where \( m^*_{e} \) is the free electron effective mass \( (1/m^*_{e} = \frac{\partial^2 \varepsilon_{e}(k)}{\partial k_z^2}) \), and in the last step we used the approximation \( |\varepsilon_k - \mu_f| \gg b(k) \). \( f(k) \) and \( g(k) \) are dimensionless functions of \( k \) where \( g(k) = 2 \text{ sign}(\varepsilon_k - \mu_f) \left( |f(k)| + |A(\Omega_k)|^2 + |B(\Omega_k)|^2 \right) \) (numerical calculations show no \( k \) point where \( g(k) \) vanishes). Inverting this we get:

\[
m^*(k) \approx m^*_{e} \left[ \Theta(\mu_f - \varepsilon(k)) + \Theta(\varepsilon(k) - \mu_f) \left(\frac{\varepsilon_k - \mu_f}{2}\right)^{2} \right]
\]

We see a similar behavior with \( Z(k) \). Again for points with \( \varepsilon_k > \mu_f \) we have quasiparticles with large effective mass, but for \( \varepsilon_k < \mu_f \) quasiparticles are free electron types and have effective mass corresponding to small, conduction electrons effective mass. We see that we have large effective mass in the points where \( Z \) is small. So indeed variations of effective mass are correlated with variations of \( 1/Z \). The approximate invariance of the product \( Z(k)m^*(k) \) is a momentum-space variant of Langreth theorem, which states that the single particle density of states in the Anderson impurity model is an adiabatic invariant, independent of the strength of the interaction.

This is interesting since it shows us that the strong angle dependent anisotropy does not apparently have large observable consequence on ordinary tunneling measurements. However it may possibly show up in the amplitude of the Friedel oscillations of the tunneling conductance around an impurity, and may therefore be accessible through Fourier transform scanning tunneling spectroscopy.

VIII. UNDERDOPED CUPRATES: PSEUDOGAPS AND FERMI ARCS IN A LARGE FERMI SURFACE METAL?

We now compare the phenomena described with observations on the normal state of the cuprate materials. As discussed above in the heavy fermion context there are portions of the Fermi surface where \( Z \sim o(1) \), and ARPES experiments may conclude that the Fermi surface consists of open ended pieces. This is strongly reminiscent of the Fermi arc phenomena reported by ARPES in the pseudogap regime of the underdoped cuprates. It is tempting therefore to imagine that a similar mechanism is operational in the cuprates. More specifically it is possible that the underdoped cuprates actually have a large band-structure-like Fermi surface but the \( Z \) is \( o(1) \) only along the observed Fermi arcs and becomes very small away from it so that those portions are not easily observed? The antinodal pseudogap itself must then be associated with a gap in the incoherent part of the electron spectrum with the gapless coherent part not resolved due to the smallness of \( Z \).

In considering this question we first observe that in the heavy fermion system the smallness of \( Z \) goes hand-in-hand with the largeness of effective mass. More generally the effective mass is not directly related to \( Z \) (it is only in cases where the electron self energy is momentum independent that \( Z \) determines the mass renormalization). So phenomenologically we need to first suppose that the small \( Z \) antinodal regions do not have mass enhancement.
Such a Fermi liquid state for the pseudogap regime has some attractive features. Consider first the gapless Fermi arcs. Several popular theories attempt to view the arcs as part of a true Fermi surface which consists of small closed hole pockets whose back portions are not observed in ARPES due to a small $Z$. However, the observed Fermi arc coincides with band structure Fermi surface and shows no tendency to bend away into a closed hole pocket. In contrast in the state discussed above the true Fermi surface is simply the band structure one but the antinodal sections would be unobservable due to a small $Z$.

Consider next recent observations of quantum oscillations at high fields and low temperatures in some underdoped cuprates. The oscillation frequency seems consistent with a small Fermi pocket. A key issue is to reconcile this with the Fermi arcs reported in photoemission, and a few different ideas have been proposed. An interesting feature of the high field experiments is a negative Hall constant which has been interpreted as evidence for an electron pocket. RecentlyMillis and Norman have proposed that the oscillations and negative Hall constant should be with a 1/8th filling antiphase stripe order, which folds the band structure Fermi surface to create a pocket. One issue with the proposal is that the electron pocket is near the edges of the full Brillouin zone - precisely the region where a big pseudogap is seen by ARPES in zero field in the normal state above $T_c$. For the theory of Ref. 24 to apply it is apparently necessary that the 60$f$ fields used in the quantum oscillation experiment wipe out the pseudogap. This may seem unnatural but is not prohibited. This difficulty is overcome in the large Fermi surface pseudogap envisaged in this section. A low temperature 1/8 antiphase stripe instability arising from that state will have retain all the same transport properties as that in the theory of Ref. 24. This is because the smallness of $Z$ does not affect transport phenomena. On the other hand the ARPES pseudogap (which in this state is the gap of the incoherent part of the spectrum) will survive intact. Thus this kind of large Fermi surface state provides a possible route to a reconciliation between the quantum oscillation and ARPES experiments.

However a number of difficulties exist with the idea that the pseudogap state has a large Fermi surface state with strong angle dependent $Z$. First, the density of states as measured by thermodynamic measurements actually decreases on entering the pseudogap state by cooling. This requires that the effective mass at the antinodal regions is suppressed (rather than enhanced) in the pseudogap state which is rather unnatural. Besides such behavior should signal an increase in the Drude weight in optical transport in the pseudogap state which is not seen. Finally this is also inconsistent with the scaling of the superfluid density with the density of doped holes.

In light of these difficulties it seems unlikely that a Fermi liquid state with a large Fermi surface of the kind discussed here is a serious candidate for the pseudogap state. These difficulties may perhaps be overcome by a non-Fermi liquid version which retains the large Fermi surface and the strong variation of the low energy spectral density. However a description of such a state does not currently exist.

**IX. DISCUSSION**

The most interesting conclusion from this work is the possibility of large variations in the quasiparticle weight (and concomitantly the effective mass) on moving around the Fermi surface. This variation is related to the internal orbital structure of the Kondo resonance, derived from the $f$-symmetry of the orbitals occupied by the local moments. In the hybridization mean field theory the most dramatic variation occurs when there are ‘hybridization nodes’, i.e., directions along which the hybridization vanishes. We demonstrated the possibility of such nodes in a simple model of a $Ce$-based cubic heavy fermion system. Hybridization nodes lead to the possibility that some portions of the large Fermi surface are actually contained within the original small Fermi surface of the conduction electrons. In those regions the quasiparticles essentially have $f$-electron character with very little admixture to the $f$-fermions. The quasiparticle weight is correspondingly large (of order 1). The opposite is true in other portions where the quasiparticles mostly have $f$-character and have small $Z$. This then leads to a strong angle dependence of the quasiparticle weight.

Real heavy electron materials have much more complicated band structures than in the simplified model considered here. Nevertheless there exists in general the possibility of hybridization nodes which will greatly affect their low temperature physics. Consider for instance heavy electron superconductivity. At least in some cases the superconductivity may be driven by formation of singlet bonds between neighbouring local moments due to RKKY interactions. In combination with Kondo hybridization this leads to superconductivity. Formally the singlet formation may be described as $<ff>$ pairing while the Kondo hybridization has non-zero $<c^\dagger f>$. This then leads to non-zero $<cc>$, i.e., superconducting order.

If the hybridization has nodes then this will lead to extra nodes in the physical superconducting order parameter over and above any nodes inherited from the singlet bond $<ff>$ amplitude.

The large variation of the $Z$ also has potential implications for current thinking on the nature of the quantum critical point between the heavy Fermi liquid and the antiferromagnetic metal. It has been suggested that this transition is accompanied by the loss of Kondo screening resulting in a reconstruction of the Fermi surface. Such a reconstruction presumably requires $Z$ to vanish through out the large Fermi surface on approaching the transition from the paramagnetic side. For a discussion on $Z$ vanishing at the heavy Fermion quantum critical points see. The variation of $Z$ described in this pa-
per raises the question of whether the manner in which Z vanishes also varies around the Fermi surface.

We also explored the possibility that the pseudogap state of the underdoped cuprates may be a large fermi surface Fermi liquid state with a strongly angle dependent Z. While such a picture has some very appealing features it has enough difficulties with experiments that it is unlikely to directly be a relevant theory of the pseudogap state.

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APPENDIX A: CALCULATION OF MATRIX ELEMENT

To calculate \( \langle \mathbf{k}, \sigma | k, M \rangle \), we use the known overlap of \( |k, J_\sigma \rangle \) for \( l = 3 \):

\[
\langle \mathbf{k}, \sigma | k, J_\sigma \rangle = 4\pi \left[ \alpha_{J_\sigma} Y_3^{J_\sigma+\frac{1}{2}}(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + \beta_{J_\sigma} Y_3^{J_\sigma-\frac{1}{2}}(\Omega_k) \delta_{\sigma, \frac{1}{2}} \right] \tag{A1}
\]

where \( Y_l^m(\Omega_k) \) are associated Legender functions and \( \alpha_{J_\sigma} = \left[(7 + 2J_\sigma)/14\right]^{1/2} \) and \( \beta_{J_\sigma} = \left[(7 - 2J_\sigma)/14\right]^{1/2} \) are Clebsch-Gordan coefficients.\(^{33}\) Now using the forms given in \( \text{[1]} \) we get the following for the two orbital states:

\[
\langle \mathbf{k}, \sigma | 1 \rangle = \frac{1}{\sqrt{6}} \left[ \frac{1}{\sqrt{7}} Y_3^{-2}(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + \sqrt{\frac{6}{7}} Y_3^{-3}(\Omega_k) \delta_{\sigma, \frac{1}{2}} \right] \\
- \sqrt{\frac{5}{6}} \left[ \sqrt{\frac{5}{2}} Y_3^{2}(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + \sqrt{\frac{2}{7}} Y_3^{1}(\Omega_k) \delta_{\sigma, \frac{1}{2}} \right]
\]

\[
\langle \mathbf{k}, \sigma | 2 \rangle = \frac{1}{\sqrt{6}} \left[ \sqrt{\frac{6}{7}} Y_3^{3}(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + \frac{1}{\sqrt{7}} Y_3^{2}(\Omega_k) \delta_{\sigma, \frac{1}{2}} \right] \\
- \sqrt{\frac{5}{6}} \left[ \sqrt{\frac{2}{7}} Y_3^{-1}(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + \sqrt{\frac{5}{2}} Y_3^{-2}(\Omega_k) \delta_{\sigma, \frac{1}{2}} \right]
\]

It is more convenient to work with a simplified version of these relations as:

\[
\langle \mathbf{k}, \sigma | 1 \rangle = \frac{1}{\sqrt{42}} \left[ Y_3^{-2}(\Omega_k) - 5 Y_3^{-3}(\Omega_k) \right] \delta_{\sigma, -\frac{1}{2}} \\
+ \frac{1}{\sqrt{42}} \left[ \sqrt{6} Y_3^{-2}(\Omega_k) - \sqrt{10} Y_3^{1}(\Omega_k) \right] \delta_{\sigma, \frac{1}{2}}
\]

\[
\langle \mathbf{k}, \sigma | 2 \rangle = \frac{1}{\sqrt{42}} \left[ \sqrt{6} Y_3^{3}(\Omega_k) - \sqrt{10} Y_3^{-1}(\Omega_k) \right] \delta_{\sigma, -\frac{1}{2}} \\
+ \frac{1}{\sqrt{42}} \left[ Y_3^{2}(\Omega_k) - 5 Y_3^{-2}(\Omega_k) \right] \delta_{\sigma, \frac{1}{2}}
\]

If we introduce new functions \( A(\Omega_k) \) and \( B(\Omega_k) \):

\[
\langle \mathbf{k}, \sigma | 1 \rangle = A(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + B(\Omega_k) \delta_{\sigma, \frac{1}{2}}
\]

\[
\langle \mathbf{k}, \sigma | 2 \rangle = -B^*(\Omega_k) \delta_{\sigma, -\frac{1}{2}} + A^*(\Omega_k) \delta_{\sigma, \frac{1}{2}} \tag{A2}
\]

where \( A(\Omega_k) = \frac{4\pi}{\sqrt{42}} \left[ Y_3^{-2}(\Omega_k) - 5 Y_3^{-3}(\Omega_k) \right] \) and \( B(\Omega_k) = \frac{4\pi}{\sqrt{42}} \left[ \sqrt{6} Y_3^{-2}(\Omega_k) - 5 Y_3^{1}(\Omega_k) \right] \).

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