Heat Transport and the Nature of the Order Parameter in Superconducting $UPt_3$

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Recent thermal conductivity data on the heavy fermion superconductor $UPt_3$ have been interpreted as offering support for an $E_{2u}$ model of the order parameter as opposed to an $E_{1g}$ model. In this paper, we analyze this issue from a theoretical standpoint including the detailed effects of Fermi surface and gap anisotropy. Our conclusion is that although current data put strong constraints on the gap anisotropy, they cannot definitively distinguish between these two models. Measurements on samples of varying quality could be decisive in this regard, however.

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Well over a decade after the discovery of heavy fermion superconductivity, the pairing mechanism and even the order parameter symmetry in these compounds remain controversial. Early suggestions of pairing in an unconventional superconducting state, based primarily on analysis of transverse ultrasound measurements in $UPt_3$, were bolstered more recently by the discovery of a complex phase diagram for this system in applied magnetic field and pressure. (Here we take “unconventional” to imply the existence of additional broken symmetries beyond the usual gauge U(1) broken in classic superconductors.)

Several current Ginzburg-Landau (GL) theories of the $UPt_3$ phase diagram attribute the existence of multiple superconducting phases to two nearly degenerate superconducting states, either (i) split by a symmetry-breaking field, such as the ordered antiferromagnetic moment in the basal plane, or (ii) “accidentally” degenerate. Such theories can at the same time describe qualitatively the anisotropy of the superconducting state, insofar as the GL parameters can be chosen to stabilize an order parameter at low temperatures and fields which allows for a larger number of quasiparticle excitations with wave vector in the basal plane. Such a state is strongly indicated by analyses of both ultrasound and thermal conductivity measurements. Beyond this crude statement, little is known for certain about the exact anisotropy or even the symmetry of the superconducting state of $UPt_3$.

Recently, Lussier et al. have argued that thermal conductivity measurements can shed further light on these questions. They showed that the electronic heat current dominates the phononic current down to low temperatures for their high quality samples, and that the relaxation rate $1/\tau_b$ in the normal state is nearly isotropic. Furthermore, their measurements imply the existence of large anisotropy in the superconducting state which does not simply reflect normal state anisotropy: together with transverse ultrasound measurements, these data provide convincing evidence for a highly anisotropic gap in $UPt_3$.

In order to determine the actual gap anisotropy for $UPt_3$, it is necessary to go further and attempt to model the data. While it has been stated that such fits to transport properties cannot be expected to fix the detailed anisotropy due to uncertainties in the form of the impurity scattering amplitude, Fledderjohann and Hirschfeld argued recently that ratios of transport coefficients should lead to more robust conclusions since they can depend only weakly on the relaxation times. They therefore focussed on the ratio $\kappa_c/\kappa_b$ between the conductivities measured for heat currents directed along the c– and b–axes, respectively, comparing the data of Lussier et al. to weak-coupling BCS calculations using order parameters representative of the $E_{1g}$ and $E_{2u}$ symmetry classes of the $D_{6h}$ space group of the hexagonal crystal. While both states have lines of order parameter nodes (and hence higher density of excited quasiparticles) in the basal plane, the $E_{2u}$ state has point nodes along the c-axis where the order parameter vanishes quadratically, in contrast to the linear behavior in the $E_{1g}$ state. In consequence, the thermal conductivity (and indeed all current-current correlation functions) was found to be isotropic in the $E_{2u}$ state over a spherical Fermi surface, despite the intrinsic anisotropy of the superconducting state. Ellipsoidal Fermi surfaces do not change the value of the normalized conductivity ratio $(\kappa_c/\kappa_{Nc})/(\kappa_b/\kappa_{N})$ from unity in this state ($N$ refers to the normal state), but it is clear that the true hexagonal crystal structure will do so. Furthermore, is not clear whether this result is specific to the $E_{2u}$ state analyzed, or would hold for a more general $E_{2u}$ state. Understanding the extent to which these factors might improve the agreement with the large measured anisotropy is crucial to the $E_{2u}$ scenario proposed by Sauls and Norman in which several problems characteristic of GL theories of type (i) above are resolved.

In this paper, we study the influence of both Fermi surface anisotropy and gap anisotropy on superconducting state transport coefficients, focussing on the thermal conductivity data of Lussier et al. In the first part, we use a simple ellipsoidal Fermi surface fit to normal state transport data and analyze all gap functions represented by ellipsoidal harmonics up through $L=5$, treating various impurity scattering rates, impurity phase shifts,
and inelastic scattering effects. First, we find that a finite, non-zero $T=0$ value of the thermal conductivity ratio, $\kappa_c(0)/\kappa_b(0)$, of intrinsic origin occurs for a number of harmonics, not just those of $E_{2u}$ symmetry. Second, we find that the data can be fit reasonably well by gaps of both $E_{1g}$ and $E_{2u}$ symmetry, with the latter fitting slightly better than the former, although in neither case is a pure harmonic realized. These fits could be differentiated more clearly by (1) extending the measurements to lower temperatures or (2) by increasing or decreasing the impurity scattering rate, that is, by analyzing cleaner or dirtier samples. Although fits using ellipsoidal harmonics may be somewhat unrealistic, they allow us to obtain some useful analytical results, and determine the qualitative features of order parameter anisotropy with some confidence.

In the second part, we turn to the more general case, using the multi-sheeted Fermi surface predicted from local density approximation (LDA) calculations which is in reasonable agreement with deHaas-vanAlphen (dHvA) experiments, up to an overall mass renormalization. Two types of gap functions are analyzed: Fermi surface harmonic and tight binding. In neither case is an adequate fit found to the data for either $E_{2u}$ or $E_{1g}$ with single basis functions, although one of the tight binding gap functions of $E_{1g}$ symmetry has some promise. In the Fermi surface harmonic case, this poor agreement is due to the large number of nodes these functions possess which is unlikely to arise out of any microscopic gap equation. In the tight binding case, this is likely due to the use of a single basis function. Use of a mixed basis set in the tight binding case leads to a good correspondence to the data in the $E_{1g}$ case. So far, we have not found a comparably good fit for the $E_{2u}$ case.

I. ORDER PARAMETERS AND Fermi Surfaces

Although a variety of models have been proposed for the order parameter of $UPt_3$, we concentrate here on the most popular model, that of a two-dimensional group representation. The two variants most commonly explored have been the $E_{1g}$ model and the $E_{2u}$ model. For a spherical Fermi surface, the gap function can be represented by spherical harmonics. A function of $E_{1g}$ symmetry first occurs in the $L=2, M=1$ representation (d-wave). The $E_{2u}$ case is more subtle since it is an odd parity gap and therefore a pseudo-spin triplet. The proposed $E_{2u}$ model assumes that the gap is a pure spin triplet with only one component ($S_z = 0$) condensed, however. In this case, $E_{2u}$ first occurs for $Y_{32}$ (f-wave). The $E_{2u}$ model based on $Y_{32}$ was originally proposed since (i) its nodal structure was similar to the previously considered $E_{1g}$ model based on $Y_{21}$, with line nodes perpendicular to the c-axis and point nodes along the c-axis as indicated by transverse ultrasound as well as point contact spectroscopy, and (ii) it has an upper critical field anisotropy consistent with experimental data given the $S_z = 0$ orientation of the triplet order parameter, as demonstrated earlier by Choi and Sauls (singlet order parameters give an incorrect anisotropy). Sauls in turn showed that this model solved a major problem of the previously considered $E_{1g}$ model, in that it could explain the existence of a tetracritical point in the H-T phase diagram for all orientations of the magnetic field as observed experimentally, at least for axial symmetry. Recently, Park and Joynt have proposed that $E_{1g}$ can avoid the problem of an incorrect upper critical field anisotropy if the normal state Pauli susceptibility has opposite anisotropy to the observed normal state susceptibility (the latter likely being van Vleck dominated). It can also give a phase diagram which has a near tetracritical point for certain choices of the GL coefficients, with the additional claim that it gives a better explanation of the pressure-temperature phase diagram than $E_{2u}$.

A potential method of resolving these controversies would be to obtain more knowledge of the actual form of the gap anisotropy. The $E_{1g}$ model has a linear dispersion of the quasiparticle energies about the point nodes, whereas the $E_{2u}$ model has a quadratic dispersion. This can have a significant effect on transport quantities, as pointed out by Yin and Maki. Fledderjohann and Hirschfeld exploited this to show that the thermal conductivity anisotropy ratio, $\kappa_c(0)/\kappa_b(0)$, is small for the $E_{1g}$ case (it would be zero in the clean limit), but is unity for the $E_{2u}$ case, at least for an ellipsoidal Fermi surface, with the data of Lussier et al lying between these two results but being more consistent with $E_{1g}$ than $E_{2u}$. This in turn motivated Lussier et al to take data at lower temperatures, where they conclude that the extrapolated $T=0$ anisotropy ratio of about 0.5 is probably intrinsic and thus consistent with an $E_{2u}$ model.

The above analysis of Fledderjohann and Hirschfeld was based on a particular spherical harmonic form of the order parameter on an ellipsoidal Fermi surface. For a real metal like $UPt_3$, we would expect that the actual order parameter is more complicated, just as we know that the actual Fermi surface is multi-sheeted and shows strong deviations from axial symmetry. The latter is particularly important since the $E_{2u}$ result $\kappa_c/\kappa_b = 1$ is a consequence of axial symmetry.

To analyze this in more detail, we first consider the simple ellipsoidal case treated previously, but look at other harmonics besides $Y_{21}$ and $Y_{32}$. The conversion from spherical to ellipsoidal harmonics can be achieved by replacing $\sin(\theta)$ by $\sin(\theta)/\sqrt{m_r}$ and $r^2$ (previously unity) by $\cos^2(\theta) + \sin^2(\theta)/m_r$, where the mass ratio, $m_r = m_L/m_\perp$, is equal to 2.8 based on normal state transport data. Note that this conversion simply multiplies $Y_{21}$ and $Y_{32}$ by an overall constant, so the results for these two cases are independent of the mass ratio. This is not true in general. For the $E_{1g}$ case, the next higher harmonic to consider is $Y_{31}$; for the $E_{2u}$ case...
\( S_z = 0 \), \( Y_{52} \). Although such higher harmonics seem exotic, they do play a significant role in certain microscopic theories. \(^{23}\)

For the real Fermi surface case, we utilize the surface obtained from an LDA calculation. \(^{11,23}\) This surface, which is shown in symmetry planes of the zone in Fig. 1, is in reasonable agreement with dHvA data, except for mass renormalization effects. The mass renormalization would play no role here unless it was anisotropic. Unfortunately, there is not enough data available to model this anisotropy, although the lack of observation of dHvA orbits for fields along the \( c \) axis suggests that the renormalization is anisotropic and will act to increase the mass ratio for fields along the \( c \) axis indicates that the renormalization, although the lack of observation of dHvA or-

The mass renormalization obtained from an LDA calculation. \(^{11,26}\) This surface, cannot be determined outside the context of a microscopic theory of the superconductivity. In fact, the gap function on independent sheets of the Fermi surface cannot be determined at each \( k \) point or, even a momentum dependence of the mass renormalization. That is, the modulus of the \( E_{1g} \) gap is \( v_{1g} \), and the \( E_{2u} \) gap \( v_r^2 \) where \( v_r^2 = v_o^2 + v_c^2 \). \(^{25}\) The nodal structure of these functions are very complicated given the complicated Fermi surface geometry. There are many points on the Fermi surface where the velocity vector points either along or perpendicular to the \( c \)-axis. In any of these cases, the \( E_{1g} \) and \( E_{2u} \) Fermi surface harmonics will vanish.

An alternate set of basis functions can be generated by tight binding expansion. In the square lattice case, the lattice vectors of type \((1,0)\) lead to a \( d \)-wave state of the form \( \cos(k_x) - \cos(k_y) \), which is currently the leading model being explored for high temperature cuprates. For the hexagonal closed packed case, \( E_{1g} \) and \( E_{2u} \) first appear for primitive lattice vectors of the type \((0,1,1)\). These can be generated from the next near neighbor basis functions listed by Putikka and Joynt \(^{14}\) by multiplying their \( E_{1u} \) and \( E_{2g} \) functions by \( \sin(k_zc) \). They are for \( E_{1g} \):

\[
f_1 = \sqrt{2} \sin(k_zc) \cos(2k_ya) \sin(\sqrt{3}k_xa)
\]

\[
f_2 = \frac{2}{\sqrt{6}} \sin(k_zc)(\sin(k_ya) + \cos(1/2k_ya)\cos(\sqrt{3}k_xa)) \quad (1)
\]

and for \( E_{2u} \):

\[
f_1 = \frac{2}{\sqrt{6}} \sin(k_zc)(\cos(k_ya) - \cos(1/2k_ya)\cos(\sqrt{3}k_xa))
\]

\[
f_2 = \sqrt{2} \sin(k_zc) \sin(1/2k_ya)\sin(\sqrt{3}k_xa) \quad (2)
\]

with a gap modulus of \( \sqrt{f_1^2 + f_2^2} \) for an assumed gap of the form \( f_1 + if_2 \) (the \( 1,i \) state). Both functions have line nodes in the \( k_z = 0 \) and \( k_z = \pi/c \) planes. In addition, the \( E_{1g} \) function has point nodes with linear dispersion along all three symmetry axes \((\Gamma - A, M - L, K - H)\), whereas \( E_{2u} \) has quadratic point nodes along \( \Gamma - A \) and linear point nodes along \( K - H \). We note that the basis functions listed by Putikka and Joynt for the near neighbor case are not properly invariant under reciprocal lattice translations due to the non-symmorphic nature of the \( UPt_3 \) lattice (that is, the near neighbors are separated by a non-primitive translation vector). This problem has been addressed by Konno and Ueda. \(^{13}\) Under the highly simplistic assumption that the phase of the single particle wavefunctions on the two sites in the unit cell is determined by a simple near neighbor interaction, they were able to generate analytic near neighbor basis functions which have proper translational symmetry. In this paper, we use their \( \Gamma_6^+ \) \( (E_{1g}) \) and \( \Gamma_5^- \) \( (E_{2u}) \) basis functions. These, in fact, can be generated from the tight binding basis functions discussed above by replacing \( \sin(k_zc) \) by \( \sin(k_zc/2) / |\phi| \) where \( \phi \) is the Fourier transform of the near neighbor distance vectors projected onto the basal plane.

\[
\phi = \frac{1}{\sqrt{3}}(e^{i\kappa_ya} + 2 \cos(k_ya/2)e^{-i\kappa_ya}) \quad (3)
\]
(φ is complex since the lattice is non-symmetric). The effect of this is to remove the line nodes in the $k_z = \pi/c$ plane and the linear point nodes along $K - H$.

## II. THERMAL CONDUCTIVITY

The thermal conductivity $κ$ in the presence of impurities is evaluated using a Kubo formula for the heat-current correlation function as in the original treatment for an s-wave superconductor by Ambegaokar and Tewordt. This treatment was generalized to unconventional states by several groups, giving results for a spherical Fermi surface and model p- and d-wave states which agreed qualitatively with experiment. Even for odd parity states, such corrections vanish in the unitarity limit. For the diagonal thermal conductivity tensor one obtains

$$
\frac{κ_i(T)}{κ_{N,i}(T)} = \int_0^\infty \frac{dw}{π} \frac{(ω)^2}{(\omega/πT)^2} \text{sech}^2 \left( \frac{ω}{2T} \right) K_i(ω, T) \tag{6}
$$

$$
K_i(ω, T) = \frac{1}{ω''} \text{Re} \int \frac{dS_k}{v_k} \frac{v_{ki}^2}{|v_k|^2} \frac{ω''}{ω''^2 - 2|Δ_k|^2} \tag{7}
$$

where $ω'$ and $ω''$ are the real and imaginary parts of $ω$, and $Γ ≡ Γ/(1 + c^2)$ is the normal state scattering rate. Here $dS_k$ is the area measure on the Fermi surface, and $v_k$ is the Fermi velocity.

For a complete description of the data, we must take into account the effects of inelastic scattering. This is known to vary as $bT^2$ times the elastic rate in the normal state, with $b ≈ 4/K^2$. This effect can be included in the above equations by replacing $Γ$ by $Γ(1 + bT^2)$. In the superconducting state, we can make the ansatz that the inelastic rate varies as $bT^3/T_c$ since the number of quasiparticles varies as $T/T_c$ at low temperatures due to the line nodes in the gap. The exact form of this makes little difference, since by far the largest effect inelastic scattering has is on $κ_N(T)$. Therefore, for practical purposes when comparing to data normalized to its value at $T_c$, one can simply scale the result of Eq. 6 by $(1 + bT^2)/(1 + bT^2)^2$.

Finally, we note that $UPt_3$ has a split superconducting phase transition. In the $E$ models considered here, this splitting is assumed to be due to the weak antiferromagnetism which has orthorhombic symmetry. Its effect is to cause only one of the two $E$ components to condense at the upper phase transition. Thus, in the region between the upper ($T_{c+} = 0.50K$) and lower ($T_{c-} = 0.44 K$) transitions, the point nodes along the $c$ axis become line nodes perpendicular to the basal plane. This explains the lack of gap anisotropy in the thermal conductivity observed in this region. Below $T_{c-}$, the second $E$ component condenses, and the anisotropy begins to occur, as observed. Modeling this is complicated since the calculation would have to be performed for orthorhombic symmetry with two different gaps and appropriate domain averaging performed. We therefore take the approach of previous work which ignores this symmetry breaking but normalizes $κ_i/κ_b$ to its value at $T_{c-}$. This normalization does not work so well, though, when comparing to the individual $κ_i(T)/T^2$ themselves, since the thermal conductivity does change above $T_{c-}$. We have found that normalizing $κ_i(T)/T$ to its value at $T_{c0} = 0.47K$, the average of $T_{c+}$ and $T_{c-}$ (the “hexagonal” $T_c$), works quite well in this regard. Obviously, one cannot take too seriously the results in the immediate vicinity of $T_c$ until the effects of the symmetry breaking field are properly included.
III. RESULTS

A. Ellipsoidal harmonics

Results for $\kappa_c/\kappa_b$ are shown in Fig. 2 for all harmonics through $L=5$ on an ellipsoidal Fermi surface with $m_r = 2.8$, compared to the experimental results of Lussier et al. [10] This quantity is normalized to its value at $T_c$ as discussed above. The results were generated with an impurity scattering rate in the unitarity limit of 0.1 $T_c$, consistent with experimental data (particularly with the observation of a residual linear specific heat coefficient of 0.16 the normal state value). [11] To understand these results more clearly, we have analytically calculated

$$\frac{\kappa_c(0)}{\kappa_b(0)} = \lim_{\omega \to 0} \frac{\text{Re}(\int_0^\omega \sqrt{\omega^2 - \Delta_T^2})}{\text{Re}(\int_0^\omega \sqrt{\omega^2 - \Delta_T^2})}$$ (8)

in the clean limit for a spherical Fermi surface, and show these results in Table 1. We see that harmonics of the form $Y_{LL}$, which have only point nodes along the $c$ axis, give a divergent ratio. On the other hand, only two of the remaining harmonics, $Y_{10}$ and $Y_{20}$, give a ratio of zero (the non-zero value in Fig. 2a is due to impurity-induced gaplessness [8], with the rest giving an intrinsic non-zero ratio. In particular, we note that harmonics of the form $Y_{L0}$ only have line nodes, so a finite, non-zero ratio is not something just associated with quadratic point nodes or with gaps of $E_{2u}$ symmetry. We also note that no pure harmonic provides a good fit to the observed anisotropy, [24] although some higher harmonics give adequate fits.

To study this further, we have looked into the possibility of mixed solutions. For $E_{1g}$, we included mixing of $Y_{21}$ with $Y_{11}$; for $E_{2u}$, $Y_{32}$ with $Y_{22}$. [33] Typical results for $\kappa_c/\kappa_b$ are shown in Fig. 3a, with the coefficients roughly optimized to fit the data. Both fits give a reasonable description of the data, with the lowest temperature data intermediate between the two results (it should be remarked that the error bars on the experimental $\kappa_c/\kappa_b$ are about 15% at low temperature [10]). The $E_{1g}$ fit can be greatly improved at lower temperature by going to a larger scattering rate of 0.3 $T_c$, but the individual $\kappa_i/T$ in this case are in poor agreement with experiment. Altering the scattering phase shift from the unitarity value of $\cot(\delta_0)$ of 0 to 0.2 slightly improves things at the lowest temperatures, but this is probably not significant given the experimental error bars. For the $E_{2u}$ case, lowering the scattering rate by a factor of ten only slightly suppresses the ratio and only for temperatures below where experimental data exist (the same slight suppression also occurs by increasing $\cot(\delta_0)$). In Fig. 3b, we compare these fits to the individual $\kappa_i/T$, normalized to their value at $T_{c0}$ as discussed previously. As can be seen, both $E_{1g}$ and $E_{2u}$ provide good fits to the data, with the $E_{2u}$ fit being slightly superior. An interesting point is that the experimental $\kappa_i/T$ are linear in temperature down to the lowest measured temperatures. This behavior cannot continue indefinitely since $\kappa_i/T$ would be zero at a temperature larger than zero (that is, $\kappa_i/T$ must flatten off). The calculated curves, though, predict that this flattening should occur in the measured temperature range in contradiction with experiment. As suggested by the authors of Ref. [10], the calculated low temperature behavior can be improved by reducing $\Gamma$ to roughly one tenth its normal state value. Although this does improve the fit at low temperatures, it leads to a substantial deviation from the data at higher temperatures. In fact, we have found that the value $\Gamma/T_c \sim 0.1$ (the normal state value) gives roughly the best fit over the entire temperature range below $T_c$. We have also found that altering the scattering phase shift from the unitarity value of $\pi/2$ does not improve the fit in this regard, at least for small values of $\cot(\delta_0)$. If this discrepancy between the low temperature and high temperature behavior is taken at face value, a strong temperature dependence of either $y = \cot(\delta_0)$ or $\Gamma$ must be assumed. Although dynamical scattering effects could easily influence the phase shifts in this way, we have been unable to find a satisfactory phenomenological explanation of the data in these terms. While a $T$-dependent parametrization of $\Gamma$ could possibly account for the discrepancy, we have no physical understanding of how such effects could arise.

The gap functions in the $E_{1g}$ and $E_{2u}$ cases are plotted as a function of polar angle in Fig. 4. Both gap functions look similar (except for the different dispersions around the point nodes at zero degrees). This indicates that the primary determinant of the thermal conductivity is the overall shape of the gap function. We also note that the maximum gap occurs at a polar angle of 52 degrees for $E_{1g}$ and 49 degrees for $E_{2u}$. Not only are these angles close, but they are also close to the angle of 54 degrees that the vector connecting near neighbor uranium atoms makes with the $c$ axis. This could be taken as indirect evidence that the electrons in the Cooper pairs reside at near neighbor sites as would be predicted by microscopic models based on antiferromagnetic spin fluctuations.

We conclude this part by remarking that both the $E_{1g}$ and $E_{2u}$ models can explain the data. One way to more clearly distinguish between the two would be to carry the experiments to lower temperatures, although given experimental error bars, it may be difficult to conclude anything definitive. At the least, one would hope to see $\kappa_i/T$ flatten off. Perhaps a better way would be to degrade the quality of the sample. In the presence of a finite concentration of impurities, states with line nodes yield a linear term in the thermal conductivity, $\kappa_i(T) \sim T/\Delta_0$ at the lowest temperatures. For generic configurations of the thermal current $J_T$ and the line nodes, the proportionality constant is actually independent of the impurity scattering rate to leading order, yielding a universal value for the low-$T$ thermal conductivity analogous to the electrical conductivity result found by P.A. Lee. [15] In the final stages of writing, we received a paper from Graf et al. [33] in which this result was obtained independently and explored in some detail.
Because of impurity-induced gapless effects of this type, the anisotropy ratio $\kappa_c(0)/\kappa_b(0)$ is always finite even for states like $E_{1g}$, as mentioned above. In such a situation, an estimate of the anisotropy may be performed by considering Eq. 7 in the gapless regime, i.e.

$$\omega = aw + i\gamma,$$

with $a$, $\gamma$ constant. We then find $\kappa_c(0)/\kappa_b(0) = (\langle \kappa^2 \rangle_F^b)/(\langle \kappa^2 \rangle_F^b)$, with $F_k = (\gamma^2 + \Delta_k^2)^{-1/2}$.

For the $Y_{21}$ case $\langle E_{1g} \rangle$ in spherical symmetry, we find $\kappa_b(T) \sim T/\Delta_0$, $\kappa_c(T) \sim \gamma T/\Delta_0^b$, giving $\kappa_c(0)/\kappa_b(0) \approx 2\gamma/\Delta_0$ for small concentrations. The residual broadening $\gamma$ is found by solving the transcendental equation $c^2 + \gamma^2(F_k)^2 = \Gamma(F_k)$, and yields a square root dependence on concentration, $\kappa_c(0)/\kappa_b(0) \sim (\Gamma/\Delta_0)^{1/2}$ up to logarithmic corrections in the unitarity limit $c = 0$. In Fig. 5, we plot the impurity concentration dependence of the anisotropy ratio in both $E_{1g}$ and $E_{2u}$ cases for $T=0.02$ and $0.2T_c$. We note the qualitatively stronger dependence of the anisotropy ratio on impurity scattering rate for the $E_{1g}$ case as compared to the $E_{2u}$ case at low temperatures.

### B. Fermi surface harmonics

The above analysis assumes an ellipsoidal Fermi surface. The actual Fermi surface for $UPt_3$ is very complicated and could substantially alter the above conclusions. In this part, we present results using Fermi surface harmonic gap functions as described in the first section with the Fermi surface shown in Fig. 1. We again assume an impurity scattering rate of $0.1T_c$. Results for $\kappa_c/\kappa_b$ are shown in Fig. 6a and for $\kappa_i/T$ in Fig. 6b. The $E_{1g}$ case gives a fair representation of the anisotropy ratio, especially at higher temperatures. Both cases, though, predict too large $\kappa_i/T$ at lower temperatures. This occurs since the Fermi surface harmonic gap functions have a very large number of nodes. These nodes are due to the complicated Fermi surface, which has many points on it where the velocity vector is either parallel or perpendicular to the $c$ axis, either case in which the $E_{1g}$ and $E_{2u}$ Fermi surface harmonics vanish. This large number of nodes is unlikely to arise out of any microscopic gap equation since such a solution would not have an optimal condensation energy. This indicates that Fermi surface harmonics are unlikely to be useful in modeling heavy fermion superconductors. Because of this, and since the addition of higher order harmonics will not reduce the number of nodes, we have not explored using mixed Fermi surface harmonics as done in the previous subsection for ellipsoidal harmonics.

### C. Tight binding functions

We next present results for tight binding gap functions. These functions represent short range interactions in the lattice, and therefore are more likely to arise out of a microscopic gap equation than the Fermi surface harmonics. Results for the functions based on (0,1,1) type primitive lattice vectors are shown for $\kappa_c/\kappa_b$ in Fig. 7a and $\kappa_i/T$ in Fig. 7b. Although the magnitude of $\kappa_i/T$ is improved over the Fermi surface harmonic case, the anisotropy ratio is in poor agreement with experiment. We therefore turn to results using the Konno-Ueda functions based on near neighbor interactions [4] (Figs. 8a and 8b). The observed anisotropy ratio is intermediate between the $E_{1g}$ and $E_{2u}$ cases. Although $\kappa_i/T$ is too large at lower temperatures for $E_{2u}$, it is not too bad for $E_{1g}$. Perfect agreement with experiment would not be expected anyway since the above basis functions do not take into account the complicated single particle wavefunctions which occur in heavy fermions due to f orbital degeneracy and f-ligand hybridization. It is interesting to note that the near neighbor tight binding functions provide the best overall comparison to the data for those functions we have analyzed on the real Fermi surface, since this reinforces the idea of near neighbor pairing that was suggested from the ellipsoidal results above. Given this, it will interesting in the future to calculate $\kappa$ for recent microscopic models which do not involve such pairing.

As in the ellipsoidal harmonic case, to test the idea of whether a mixture of tight binding basis functions would improve the results, we have done calculations mixing the two tight binding functions considered above for each symmetry. Only a rough optimization of the mixing coefficients could be determined due to calculation demands. These results are presented in Figs. 9a and 9b. A good fit was obtained for the $E_{1g}$ case with an equal admixture of the two functions. This result is somewhat surprising since an equal admixture would imply (within a tight binding framework) that the pair interaction has a substantial range (the near neighbor separation is 7.8 a.u., but an $(0,1,1)$ vector is 14.3 a.u.). In the $E_{2u}$ case, we never found an adequate fit, although we do show a typical result (equal admixture, but with opposite sign). One should be cautious, though, about ruling against an $E_{2u}$ model based on this, since there are other functions involving non-primitive translation vectors, with distances comparable to the $(0,1,1)$ primitive vectors, which we have not considered here (one at 13.4 a.u., another at 15.2 a.u.)

### IV. CONCLUSIONS

In conclusion, we have found by analyzing simple ellipsoidal models for the Fermi surface that recent thermal conductivity data cannot unambiguously differentiate between the $E_{1u}$ and $E_{2u}$ models for the symmetry of the order parameter. Such a differentiation should be possible by looking at samples with degraded quality, since in the $E_{2u}$ case, the non-zero value of $\kappa_c(0)/\kappa_b(0)$ is intrinsic, whereas for $E_{1g}$, it is due to impurities. We have also
found that results using realistic Fermi surfaces and gaps with proper lattice translational symmetry differ significantly from those based on ellipsoidal Fermi surfaces, and have discovered an $E_{1g}$ tight binding gap function which gives a good representation of the data. We emphasize that the thermal conductivity data appear to put great constraints on the overall shape of the gap function, and thus will be an important ingredient in determining the validity of microscopic models for the superconductivity in $UPt_3$.

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The analysis in this paper was greatly facilitated by the analytic nature of the basis functions. Most microscopic models, such as the one in Ref. [23], are numerical and thus more difficult to treat given the large number of tetrahedra needed in the zone integrations.

| L M  | Form                              | m_r=1 | m_r=2.8 |
|------|-----------------------------------|-------|---------|
| 10   | cos(θ)                            | 0     | 0       |
| 11   | sin(θ)                            | ∞     | ∞       |
| 20   | 3 cos²(θ) − r²                    | 1     | 0.357   |
| 21   | sin(θ) cos(θ)                     | 0     | 0       |
| 22   | sin²(θ)                            | ∞     | ∞       |
| 30   | cos(θ)(5 cos²(θ) − 3r²)            | 6/7   | 0.423   |
| 31   | sin(θ)(5 cos²(θ) − r²)             | 1/2   | 0.180   |
| 32   | sin²(θ) cos(θ)                     | 1     | 1       |
| 33   | sin³(θ)                            | ∞     | ∞       |
| 41   | sin(θ)(7 cos³(θ) − 3 cos(θ)r²)     | 0.647 | 0.252   |
| 52   | sin²(θ)(3 cos³(θ) − cos(θ)r²)     | 0.744 | 0.267   |
| 54   | sin³(θ) cos(θ)                     | ∞     | ∞       |

**FIG. 1.** LDA Fermi surface for UPt_3 plotted in the symmetry planes of the Brillouin zone. The surface is composed of five bands, three centered around Γ and two centered around A.

**FIG. 2.** χ_c/χ_b (normalized to its value at T_c−) for various harmonics through L=5 (curves labled by L,M) on an ellipsoid (m_r=2.8). All plots, unless otherwise noted, are for an impurity scattering rate, Γ, of 0.1 T_c in the unitarity limit, with an inelastic scattering rate 4T² times the elastic rate. The black dots are data from Ref. [10].

**FIG. 3.** (a) χ_c/χ_b and (b) χ_i/T for mixed harmonics on an ellipsoid (m_r=2.8). The curve marked 1g is for E_{1g} (Y_{21} − 0.15Y_{41}) and the one marked 2u for E_{2u} (Y_{32} + 0.2Y_{52}). Black dots in (a) and black (white) dots in (b) are data from Ref. [10]. The solid (dashed) curves in (b) are the respective theoretical results for i=b (i=c).

**FIG. 4.** Order parameter versus polar angle for mixed harmonics on an ellipsoid (m_r=2.8).

**FIG. 5.** χ_c/χ_b at T/T_c = 0.02 (solid line) and T/T_c = 0.2 (dashed line) vs. normalized impurity scattering rate, Γ/T_c, for pure ellipsoidal harmonics Y_{32} (2u) and Y_{21} (1g), as well as for the mixed harmonics of Fig. 3a (2u∗ and 1g∗).

**FIG. 6.** (a) χ_c/χ_b and (b) χ_i/T for Fermi surface harmonics on the LDA Fermi surface. Same notation as Fig. 3.

**FIG. 7.** (a) χ_c/χ_b and (b) χ_i/T for tight binding functions (0,1,1 type primitive lattice vectors) on the LDA Fermi surface. Same notation as Fig. 3.

**FIG. 8.** (a) χ_c/χ_b and (b) χ_i/T for near neighbor tight binding functions (Konno-Ueda type) on the LDA Fermi surface. Same notation as Fig. 3.

**FIG. 9.** (a) χ_c/χ_b and (b) χ_i/T for mixed tight binding functions on the LDA Fermi surface. Same notation as Fig. 3.
