Origin of heavy-fermion behavior in $CeCu_2Si_2$

J.-S. Kang

Department of Physics, University of Michigan, Ann Arbor, Michigan 48109-1120
and Department of Physics and Institute for Pure and Applied Physical Sciences,
University of California at San Diego, La Jolla, California 92093

J. W. Allen

Department of Physics, University of Michigan, Ann Arbor, Michigan 48109-1120

O. Gunnarsson, N. E. Christensen, and O. K. Andersen

Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Federal Republic of Germany

Y. Lassailly

Ecole Polytechnique, 91128 Palaiseau, France

M. B. Maple

Department of Physics and Institute for Pure and Applied Physical Sciences,
University of California at San Diego, La Jolla, California 92093

M. S. Torikachvili

Department of Physics, San Diego State University, San Diego, California 92182

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We report the theoretical analysis of electron spectroscopy data for the heavy-fermion superconductor $CeCu_2Si_2$, using the impurity Anderson Hamiltonian applied to the Ce $4f$ electrons. A good description of the spectra for $CeCu_2Si_2$ is obtained, using rescaled *ab initio* hybridization matrix elements. The spectra are generally consistent with a Kondo Fermi-liquid description of this material. Near trivalence and a very small Kondo temperature are controlled more by hybridization of Ce $4f$ to Si and Cu s/p than to Cu $3d$ states.

I. INTRODUCTION

$CeCu_2Si_2$ is the original heavy-fermion superconductor[1] with superconducting transition temperature $T_c \sim 0.6$ K.[1,2] A Fermi-liquid picture[3,4] of this compound introduces a spin fluctuation, or Kondo temperature, $T_K \approx 10$ K, which has been obtained from transport and neutron scattering measurements. At temperatures sufficiently higher than T_K, the magnetic properties[5-12] are determined by well-defined local $4f$ moments, corresponding to the Ce valence close to 3+. Below T_K, a nonmagnetic Fermi-liquid state develops from the quasiparticles near the Fermi level E_F. These heavy quasiparticles probably originate from interactions between the localized Ce $4f$ electrons and the conduction electrons. At T_c, there is a phase transition from the Fermi-liquid state into the superconducting state, involving pairs of the heavy quasiparticles.

An important aspect of a heavy-fermion material[13,14] is to determine what features of its electronic structure give rise to the heavy-fermion properties, and how these features depend on the atomic constituents and the crystal structure. For Ce materials, great progress has been made recently in this task by the analysis of the $4f$ and $3d$ electron spectra, using the degenerate impurity An-

derson Hamiltonian.[15-17] In this model the $4f$ electrons occupy a local orbital of degeneracy N_f, with a binding energy ε_f relative to E_F. The Hamiltonian for this model is

$$H = \sum_{k,\sigma} \varepsilon_k n_k + \sum_{m,\sigma} \varepsilon_f n_{m\sigma} + \sum_{k,m,\sigma} (V_{km} a_{m\sigma}^\dagger a_{k\sigma} + \text{H.c.})$$
$$+ \tfrac{1}{2} \sum_{m,m',\sigma,\sigma'}{}' U n_{m\sigma} n_{m'\sigma'} .$$

The first two terms represent the conduction states and the N_f $4f$ states, labeled by m and σ. The third term describes the $4f$-conduction electron hybridization with one electron matrix element V_{km}. The fourth term describes the on-site Coulomb interaction U between two f electrons. For the $3d$ core spectrum, the Hamiltonian H' has two terms added to H,

$$H' = H + \varepsilon_c n_c - \sum_{m,\sigma} (1 - n_c) U_{fc} a_{m\sigma}^\dagger a_{m\sigma} .$$

The first term describes a core level and the second term describes the interaction between the core hole and the f electron. Using the method of the $(1/N_f)$ expansion, the various electron spectra and the static zero-temperature susceptibility $\chi(0)$ can be calculated.[15,16] Using this

theory the experimental spectra can be fit, thus determining the Hamiltonian parameters, which can then be used to calculate $\chi(0)$.[17] In a realistic theory it is necessary to include in H the spin-orbit and crystal-field splittings of the local orbital degeneracy. The latter is especially important for calculating $\chi(0)$, and a Kondo temperature T_K can then be defined by

$$T_K = \frac{C}{\chi(0)} n_f ,$$

where C is the Curie constant appropriate to the lowest-energy crystal-field term of the $4f^1$ state, and n_f is the fraction of $4f^1$ in the ground state of H.

To solve the impurity Anderson model does not require the individual hybridization matrix elements, but only the particular combinations $|V_m(E)|^2$, where

$$\sum_k V_{k,m}^* V_{k,m'} \delta(E-E') \equiv |V_m(E)|^2 \delta_{m,m'} .$$

In this model, the energy dependence of the hybridization matrix elements plays an important role.[18-20] Thermodynamic properties are essentially determined by the value of $|V(E)|^2$ close to E_F, while electron spectra are influenced by $|V(E)|^2$ over a larger energy range and so can reflect structures in its energy dependence.

In spite of the importance of CeCu$_2$Si$_2$, the impurity Anderson model analysis has been carried out only incompletely thus far.[18] In this paper we analyze in detail the Ce $3d$ spectrum obtained by x-ray photoelectron spectroscopy (XPS), the Ce $4f$ spectrum obtained by resonant photoelectron spectroscopy (RESPES), and the Ce $4f$ spectrum obtained with bremsstrahlung isochromat spectroscopy (BIS). The $4f$ RESPES data are taken from Ref. 21, while the $4f$ BIS and 3D XPS data were obtained by us as part of this study and are in good agreement with other data[22,23] in the literature. For $|V(E)|^2$ we use the result of a recent *ab initio* calculation[18] performed within the local density approximation. The m dependence of $V(E)$ is neglected, and then, as in previous work,[15-17] the hybridization strength can be characterized by its average over the conduction band, Δ_{av}, where $\Delta(E) \equiv \pi |V(E)|^2$. As discussed in the following, for the spectra it suffices to include in H only the spin-orbit splitting, but for $\chi(0)$ it is essential to include also the crystal-field splitting. The neglect of the m dependence of $|V_m(E)|^2$ may be of importance for $\chi(0)$. The calculated energy dependence of $V(E)$ leads to a good description of the spectra, if we rescale the calculated $V(E)$ by a constant factor. The ground state is then nearly trivalent, and the spectroscopic value of T_K is very small, in fact much smaller than the experimental value. To reproduce the experimental $\chi(0)$, the spectroscopic value of $V(E)$ must be increased.

The remainder of the paper is organized as follows. Section II describes experimental details, Sec. III presents the results of the impurity Anderson Hamiltonian analysis, Sec. IV discusses the implications and limits of the analysis, and Sec. V gives a summary of our conclusions.

II. EXPERIMENTAL DETAILS

The sample studied was a polycrystalline sample which was prepared by arc melting the elements, followed by annealing in argon. The crystal structure and the stoichiometry were checked by x-ray powder diffraction. The Ce $3d$ core level XPS data were obtained with non-monochromatic Al $K\alpha$ radiation. The BIS spectra were taken at a photon energy of 1486.6 eV with the Vacuum Generators ESCALAB at the Xerox Palo Alto Research Center. The sample was cooled to $T \sim 100$ K, cleaved *in situ* with a base pressure of $\sim 7 \times 10^{-11}$ Torr, and kept at the same temperature during measurement. The overall instrumental resolution is 1.2 eV for XPS and 0.6 eV for BIS. The Fermi level of the system was determined from the valence-band spectrum of a silver sample cleaned by sputtering *in situ*. The satellites in the XPS spectrum due to Al $K\alpha_{3,4}$ radiation were numerically removed.[17] The inelastic backgrounds were subtracted in such a way that the background at binding energy ε is proportional to the convolution of the primary spectrum with the inelastic loss spectrum, approximated by a step function at ε. The inelastic background to the BIS spectrum was removed by a straight line.

III. RESULTS AND DATA ANALYSIS

The top panel of Fig. 1 shows the hybridization matrix elements $|V(E)|^2$ for CeCu$_2$Si$_2$, which are used for calculating fits shown in Fig. 2. The middle and bottom panels of Fig. 1 show the Cu d and Si p partial density of states (PDOS) for CeCu$_2$Si$_2$, respectively. Each PDOS represents the contribution per spin and for two Si and Cu atoms, respectively. Note the different vertical scales for the two PDOS results. $|V(E)|^2$ was calculated using the local spin density (LSD) approximation of the density functional formalism.[18-20] These hybridization matrix elements have been corrected for the configuration dependence,[18] and are appropriate for $f^0 \to f^1$ hopping. The same matrix elements are used for $f^1 \to f^2$ hopping and for hopping in the presence of a core hole, although the matrix elements for these different processes are not the same. In applying the LSD hybridization matrix element for fitting spectra, we have to use the overall adjustment factor of $c^2 \sim 0.45$ for the hybridization matrix element, i.e.,

$$|V(E)|^2 \to c^2 |V(E)|^2 .$$

The origin of this adjustment factor is discussed in the following.

The dots in panels (a)–(c) of Fig. 2 show the experimental $4f$ BIS, $4f$ PES, and $3d$ XPS spectra, and the solid lines show the corresponding theoretical spectra, respectively. To simulate the experimental broadening, a Gaussian broadening of 1.2, 0.6, and 0.6 eV full width at half maximum (FWHM) was used for the theoretical $3d$ XPS, $4f$ PES, and BIS spectra, respectively. The Ce $3d$ XPS spectrum shows spin-orbit-split components of $3d^9_{5/2}$ and $3d^9_{3/2}$, separated by about 18.4 eV. The weight of the lowest binding energy feature, the $3d^9_{5/2} 4f^2$ shoulder, is a measure of the hybridization, while the highest
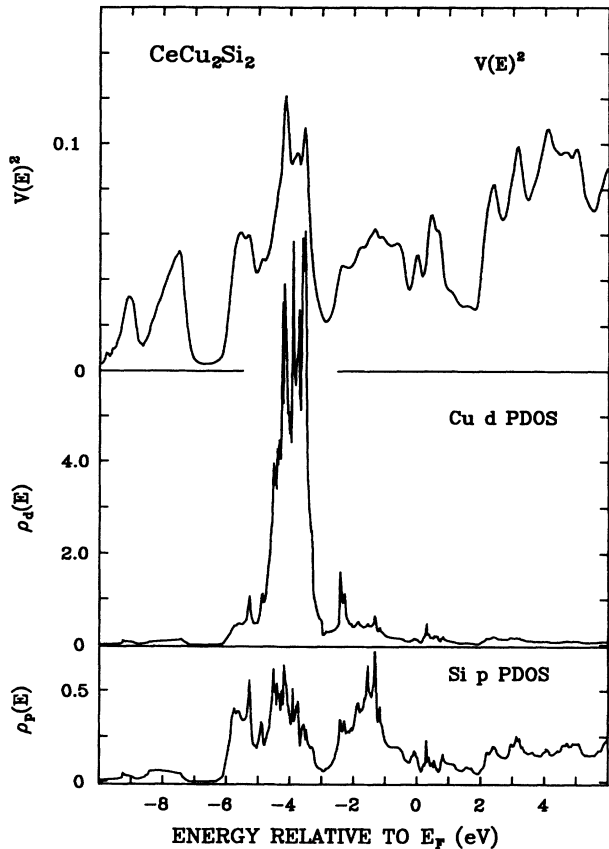
FIG. 1. Top panel: The square of the magnitude of the hybridization matrix element calculated using the local spin-density approximation for $CeCu_2Si_2$. Middle and bottom panels: Cu d and Si p partial densities of states for $CeCu_2Si_2$, respectively. These partial densities of states are per spin, and for two Cu atoms and two Si atoms, respectively.
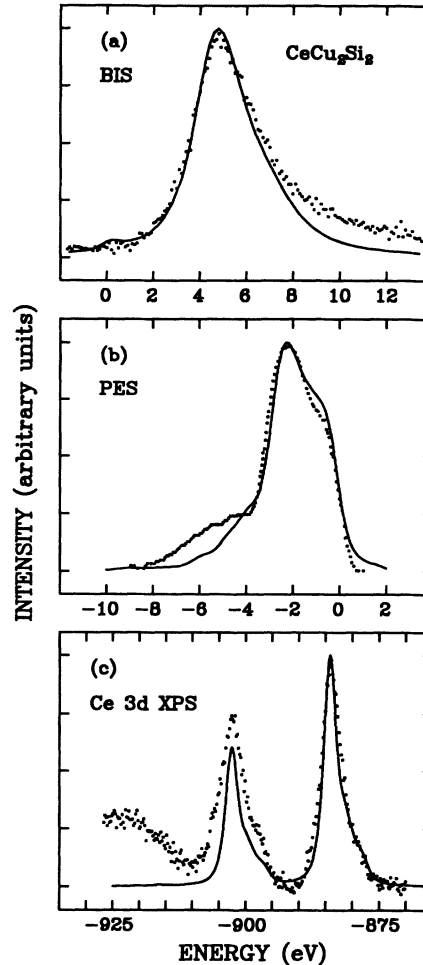

FIG. 2. Comparison of the spectrum calculated using the impurity Anderson Hamiltonian (solid lines) with the experimental spectrum (filled circles) for (a) $4f$ BIS, (b) $4f$ PES, and (c) Ce $3d$ XPS in $CeCu_2Si_2$. The experimental $4f$ PES spectrum was extracted from the data in Ref. 21.

binding energy peak, the $3d_{3/2}^9 4f^0$ peak, is a measure of the f^0 weight, i.e., approximately $1-n_f$. The f^0 weight is very small, consistent with the BIS spectrum, which has essentially no $4f$ weight near E_F. The shoulders at lower binding energy of the $3d^9 4f^1$ peaks reflect the structured energy dependence in $V(E)$. Due to the attractive Coulomb interaction between the core hole and the f electrons, the threshold of the $3d^9 4f^2 vv$ continuum lies below that of the $3d^9 4f^1 v$ continuum by such an amount that the latter is near the large Cu $3d$ peak of the former, where v denotes a valence hole. Hybridization between the two continua leads to the structured peak, which can be thought of as a structured virtual bound state.[24]

The measured BIS spectrum, shown in Fig. 2(a), is dominated by the larger Ce $4f$ weight of ~ 13 unoccupied $4f$ states, yielding the $4f^2$ peak at ~ 6 eV. The $4f$ PES spectrum, shown in Fig. 2(b), is obtained by subtracting the spectrum at the Fano minimum from that at the Fano maximum in the Ce $4f$ photoionization cross section around the Ce $4d \rightarrow 4f$ threshold.[21] These spectra are calculated using essentially the same parameters as for

the $3d$ XPS spectrum. The location of the peak at $E \sim -2.5$ eV in the theoretical PES spectrum is somewhat too low and the weight at E_F is a bit too large. This discrepancy may be due to several simplifications in the model, e.g., lattice effects not included in the impurity calculations, or the effects of higher-order terms in $(1/N_f)$. Table I summarizes the information obtained from our fits for $CeCu_2Si_2$, except for $\chi(0)$, which we dis-

TABLE I. Parameter values for $CeCu_2Si_2$.

ε_f	-2.4 eV
U	7.27 eV
U_{fc}	11.5 eV
f^0	0.011
f^1	0.956
f^2	0.033
n_f	1.022
Δ_{av}	0.059 eV

cuss next.

We have also calculated $\chi(0)$ to lowest order in $(1/N_f)$, including double occupancy of the f level, as well as spin-orbit and crystal-field splittings. For this calculation, the crystal-field splittings are those given in Ref. 6, and the parameters of H have the values determined spectroscopically, except for the scaling of $|V(E)|^2$, as described in the following. The lowest crystal-field state is a doublet for which the Curie constant has been calculated to be $C = 0.34$ emu K/mol.[7] In comparing to experiment, we have the uncertainty that the experimental values vary somewhat from sample to sample.[11] These uncertainties play a rather small role for determining what magnitude of $V(E)$ is needed to reproduce experiment. The reason for this is that CeCu$_2$Si$_2$ is in a parameter range where T_K depends exponentially on the parameters. For example, changing $|V(E)|^2$ by 3% from the value needed to reproduce the experimental $\chi(0)$ changes the calculated $\chi(0)$ by a factor of 3. Thus we have chosen as an experimental value for $\chi(0)$ the c-axis value of $\sim 20 \times 10^{-3}$ emu/mole from Ref. 2. This value corresponds to $T_K \sim 17$ K. We find that in order to reproduce this experimental $\chi(0)$ it is necessary to increase the spectroscopy value of $|V(E)|^2$ by about 40%, which changes the scale factor c^2 from its spectroscopic value of ~ 0.45 to ~ 0.63. Using the spectroscopic value of c^2 yields a value of $\chi(0)$ larger than experiment by roughly three orders of magnitude, i.e., T_K is far too small. A possible explanation for this is given in Sec. IV. It is also essential to include the crystal-field splitting. If the crystal-field splitting is set to zero, $\chi(0)$ is decreased by a factor of $\sim 10^{-3}$ for the spectroscopic value of c^2, and by a factor of ~ 0.20 for $c^2 = 0.63$. Thus the sensitivity to the crystal-field splitting is considerably larger for the smaller spectroscopic value of $V(E)$. It is entirely fortuitous that, as follows from the factors already given, the value of $\chi(0)$ with no crystal-field splitting, but using the spectroscopic value of $V(E)$, is of the same order of magnitude as the experimental value. $\chi(0)$ is also very sensitive to the inclusion of double occupancy of the f level, as discussed elsewhere.[25] Neglecting double occupancy is found to increase $\chi(0)$ by a factor $\sim 10^2$.

IV. DISCUSSION

It is of great interest to know the relative importance of hybridization to the Cu d states or to the Si p states in determining the Ce spectral features, or the thermodynamic properties. In past work[17] on fitting the spectra of binary cerium compounds, the energy dependence of $|V(E)|^2$ was taken with considerable success to be that of an off-resonance RESPES spectrum. For CeCu$_2$Si$_2$, this procedure yielded reasonable fits for the $4f$ BIS and $3d$ XPS spectra, but the $4f$ PES spectrum predicted was qualitatively wrong. The reason for this failure is that the off-resonance spectrum is dominated by the Cu d states, so that coupling to the Si p states is badly underestimated.

The average value of the hybridization strength between the Ce $4f$ and Si p states can be estimated as com-

parable to that between the Ce $4f$ and Cu d states. In general, the hybridization matrix element, $V_{l,l'}$, between orbitals of angular momentum l and l' on different sites, depends on the site separation d as[26]

$$V_{l,l'} \propto \left[\frac{1}{d} \right]^{l+l'+1} ,$$

$$\Delta \propto V_{l,l'}^2 .$$

Also, $\Delta_{l,l'}$ is assumed to be proportional to the number of near neighbors, i.e., the contributions from more distant neighbors are neglected, although these contributions are not always small. The value of $\Delta_{av} \approx 0.095$ eV for CeSi$_2$ was previously deduced from the analysis of the electron spectroscopy data,[27] in which d(Ce-Si) is 3.13 Å and Ce ion has 12 nearest-neighbor Si ions. The intermetallic compound CeCu$_2$Si$_2$ forms in the tetragonal ThCr$_2$Si$_2$ structure, where near neighbors of Ce atoms are eight Si atoms and eight Cu atoms, with the interatomic distance d(Ce-Si) = 3.13 Å, and d(Ce-Cu) = 3.22 Å, respectively. By applying the above-mentioned relations to CeCu$_2$Si$_2$ and CeSi$_2$, with l(Ce $4f$) = 3 and l'(Si $3p$) = 1, respectively, the estimated value of Δ_{av} (Ce $4f$-Si $3p$) for CeCu$_2$Si$_2$ is ≈ 0.063 eV. Similarly, using the information that $\Delta_{av} \approx 0.11$ eV for CeNi$_2$,[17] which has d(Ce-Ni) = 3.16 Å and 12 nearest-neighbor Ni ions, the estimated value of Δ_{av} (Ce $4f$-Cu $3d$) for CeCu$_2$Si$_2$ is ≈ 0.059 eV.

Our present analysis, using the *ab initio* energy-dependent hybridization matrix elements, suggests that the coupling to the Si p states is most important in determining the ground-state properties for stoichiometric CeCu$_2$Si$_2$, whereas the Ce spectral features are determined by the coupling to both the Si p and Cu d states. Structures in both ρ(Cu-d;E) and ρ(Si-p;E) are reflected in $|V(E)|^2$. For example, structures in -8 eV $< E < -4$ eV in the valence band spectrum [see Fig. 2(b)] reflect the coupling to the Cu $3d$ PDOS (see Fig. 1). Band structure calculations[28-30] for CeCu$_2$Si$_2$ show that narrow Ce $4f$ bands occur near E_F, that Si p states are broad and degenerate with the Ce $4f$ states, and that the Cu d states are very narrow, almost filled, and far below the Ce $4f$ states. Our Cu $2p$ XPS data for CeCu$_2$Si$_2$ (not shown in this paper) have only d^{10}-like peaks, also implying that the Cu d orbitals are almost filled. Even though the Cu d states have a large PDOS, the contribution to the hybridization matrix element is fairly small, because the Cu d orbitals are relatively compact. In contrast, the Si p states have a rather small PDOS, but the contribution to the hybridization matrix element is large, because the Si p orbitals are spatially extended. In consequence, for stoichiometric material the Si p PDOS dominantly contributes to the hybridization matrix element near E_F, which essentially determines the ground-state properties, such as n_f and T_K, while the Cu d orbitals are too far below E_F to influence n_f and T_K.

We have found that to describe $\chi(0)$ the magnitude of $|V(E)|^2$ must be increased by a factor ~ 1.4 relative to the value needed to fit the electron spectra. We note first that $\chi(0)$ was calculated only to lowest order in $(1/N_f)$. For a smooth $|V(E)|^2$ and without crystal-field or spin-

orbit splitting, the lowest-order calculation leads to an underestimate of $\chi(0)$.[31] A more accurate calculation of $\chi(0)$ in this case should therefore increase the deviation between the spectroscopic and thermodynamic $|V(E)|^2$. The deviation could be due to the neglect of the m dependence of $V_m(E)$. Another possible explanation is the renormalization of $V(E)$ due to the Coulomb interaction between the f electrons and the conduction electrons, which is not explicitly included in the model. A recent calculation[32] shows that the effect is expected to give a small renormalization of $V(E)$ to be used for spectroscopy properties, but that it should renormalize $|V(E)|^2$ used for thermodynamic properties by about $(E_0/T_K)^\alpha$, where $\alpha \sim 0.1$ and $E_0 \sim 1$ eV is the energy scale for $|V(E)|^2$. Because of the small value of α, this effect is rather small for compounds with $T_K \sim 0.1$ eV, while it is as large as a factor of 2 for $CeCu_2Si_2$ with $T_K \sim 1$ meV.

We further note that the calculated values of $|V(E)|^2$ have to be reduced by about a factor $c^2 = 0.45$ to describe the electron spectra. The source of this renormalization is presently unknown, but a possible reason is that the local spin density approximation gives f states that are too extended due to a potential that is not sufficiently attractive. This could be caused by the unphysical interaction of the f electron with itself in this approximation, which would cause $V(E)$ to be too large, but not greatly affect its energy dependence.

It might be thought that one or the other of the two renormalization effects is the result of neglecting the crystal-field splittings in calculating the electron spectra, but this is not the case. The large error in neglecting the crystal field is that the fractional amount of the f^0 configuration in the ground state is badly overestimated, which is why the value of $\chi(0)$ is too small. But for a small-T_K material like $CeCu_2Si_2$, the amount of f^0 is in either case so small that it does not affect the spectra, i.e., there is no f^0 peak in the $3d$ XPS spectrum, and the weight near E_F in the $4f$ spectrum is due to the f^2 component of the ground state, which depends very little on the degeneracy of the lowest f^1 configuration.[25]

V. CONCLUSION

To summarize, we have analyzed the Ce $4f$ PES/BIS and $3d$ XPS spectra of $CeCu_2Si_2$, using the impurity Anderson Hamiltonian applied to the Ce $4f$ electrons. By rescaling the energy-dependent hybridization matrix element calculated *ab initio*, a good description of the spectra is obtained, yielding near trivalence, consistent with essentially no $4f$ spectral weight near the Fermi level. To describe the static zero-temperature magnetic susceptibility, the hybridization matrix element $V(E)$ derived from the spectroscopic properties must be increased by about 20%. In broad general terms, however, and taking into account the exponential sensitivity of T_K to variations in $|V(E)|^2$, we conclude that the spectroscopic properties of $CeCu_2Si_2$ are consistent with the Kondo Fermi-liquid description of this material.

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