CeRhIn$_5$ crystallizes in the same tetragonal HoCoGa$_5$ structure as the heavy fermion superconductors CeIn$_3$ and CeCoIn$_5$. At ambient pressure, CeRhIn$_5$ undergoes a transition to an antiferromagnetic (AF) state at $T_N = 3.8$ K. With application of hydrostatic pressure, the Néel temperature remains essentially constant until antiferromagnetism disappears and superconductivity appears at pressures above 15 kbars. Recently, Pagliuso et al. have suggested a similar scheme, but with splittings 6 and 12 meV based on an analysis of the susceptibility and specific heat. An analysis of neutron scattering data for CeRhIn$_5$, which includes the magnetic susceptibility and specific heat, and IE neutron spectra. The first step in our investigations has been to determine the crystal field level scheme in CeRhIn$_5$.

In CeRhIn$_5$, as in the other members of CeMIn$_5$ family, the crystal field Hamiltonian in tetragonal symmetry can be written as

$$H_{CF} = B_{2}^{0} O_{2}^{0} + B_{4}^{0} O_{4}^{0} + B_{4}^{1} O_{4}^{1},$$

where $O_{m}^{1}$ and $B_{j}^{m}$ are the Stevens operators and CF parameters, respectively. The Ce$^{3+}$ $J = 5/2$ wave function splits into three doublets, $\Gamma_{4}^{3} = \{ \alpha \pm 5/2 \}$, $\Gamma_{7}^{2} = \{ \beta \pm 5/2 - \alpha \pm 3/2 \}$, and $\Gamma_{6}^{1} = \{ \alpha \pm 1/2 \}$. An analysis of susceptibility and thermal expansion results suggested ground state doublets.

A key problem in our investigations was the high neutron absorption of both In and Rh. In initial experiments, the standard LRMECS sample holder was used; however, in subsequent experiments a new sample holder was employed, which was designed to maintain a more uniform sample thickness than the standard holder, thus allowing for a more accurate absorption correction. Neutron scattering spectra were collected for several different incident energies ($E_i$) and temperatures between 8 and 140 K with counting times ranging from 24 to 48 h. To improve statistics, we were able to take advantage of the nondispersive nature of the CF scattering and group detectors into three bins with mean scattering angle 20° (low $Q$), 60°, and 100° (high $Q$). A vanadium standard was utilized to put the scattering on an absolute scale.

Neutron scattering results for the tetragonal compound CeRhIn$_5$ give evidence for two crystal field (CF) excitations at 6.9 and 23.6 meV. The scattering can be fit assuming a set of CF parameters $B_{2}^{0} = -1.03$ meV, $B_{4}^{1} = 0.044$ meV, and $B_{4}^{1} = 0.122$ meV. To compare our results with previous work, we calculate the susceptibility and specific heat for this CF scheme, including a molecular field term $\lambda = 35$ mol/emu to account for the Kondo effect. We also include a calculation based on these CF parameters, which uses the noncrossing approximation to the Anderson model to estimate the effect of Kondo physics on the susceptibility, specific heat, and neutron linewidths.

DOI: 10.1103/PhysRevB.66.193102 PACS number(s): 75.30.Mb, 75.20.Hr, 71.27.+a, 71.28.+d
FIG. 1. Neutron energy spectra of (a) CeRhIn₅ and (b) LaRhIn₅ at an initial energy $E_i = 35$ meV, at 8 K and for two mean scattering angles, 20° and 100°. The data have been corrected for neutron absorption, and the scattering from the sample holder has been subtracted from the data. (c) The $Q=0$ magnetic scattering, determined as described in the text, in CeRhIn₅ at 8 K and for three incident energies $E_i$.

Data for CeRhIn₅ and LaRhIn₅ (measured to help identify the nonmagnetic scattering in CeRhIn₅) at 8 K and $E_i = 35$ meV for low and high $Q$ are shown in Fig. 1. The data were corrected for absorption assuming a uniformly thick flat-plate sample, and the scattering due to the empty sample holder was then subtracted from the data. Direct comparison of low-angle scattering (where magnetic scattering is strongest) for CeRhIn₅ [Fig. 1(a)] and LaRhIn₅ [Fig. 1(b)] shows two additional peaks near 7 and 23 meV. In particular, we determine the nonmagnetic scattering in CeRhIn₅ in two ways: (1) By using the expression $S_{mag}(20°)/S(\text{Ce},20°) - fS(\text{La},20°)$ where we choose the factor $f$ as the ratio (0.75) of the total scattering cross sections $\sigma(\text{CeRhIn₅})/\sigma(\text{LaRhIn₅})$. (2) By determining the ratio $R = S(\text{La},100°)/S(\text{La},20°)$ for scaling the high angle nonmagnetic scattering to low angle. Excellent agreement with (1) is obtained using $S_{mag}(20°) = S(\text{Ce},20°) - fS(\text{Ce},100°)/R$ with inclusion of an additional factor $F = 0.75$ to account for the difference in $Q$-scaling of the La and Ce compounds. The value of $F$ is similar to the one used in a recent study of YbXCu₄₄; it can be justified on the basis that for high angle scattering the data are predominantly single-phonon, proportional to $\sigma$, while the low angle scattering contains a significant contribution from multiple scattering (one elastic and one phonon) proportional to $\sigma^2$, so that the cross section does not cancel in the ratio. Results of this analysis for three different $E_i$ are shown in Fig. 1(c). The dependence of the scattering on the Ce³⁺ form factor has been removed in this plot, so the data represent the $Q=0$ scattering with the assumption that the crystal fields are, in fact, purely local and uncoupled entities. The data have been truncated below 0.15$E_i$ (where the elastic line dominates the scattering) and above 0.8$E_i$, where statistics are small due to the $k_f/k_i$ factor. Good agreement is evident for data taken at three different $E_i$, with all datasets displaying magnetic excitations at approximately 7 and 24 meV.

In Fig. 2 we plot the $Q=0$ (form factor removed) magnetic scattering (method 1), determined at $E_i = 35$ meV for three different temperatures. We have performed a simultaneous least squares fit to four datasets (8 K, 70 K, and 140 K at $E_i = 35$ meV and 8 K at $E_i = 80$ meV) to determine the CF parameters. The fit includes the effects of instrumental resolution. Variables of the fit include $B_2^0$, $B_4^0$, $B_6^0$, and an overall scale factor (in which the four parameters were constrained to the same values for all datasets) and the Lorentzian half-width $\Gamma$ of the IE excitations, which was allowed to vary with temperature. [We constrained the quasielastic (QE) half-width to (1/2)$\Gamma$.] Results of the fit are shown in Table I and plotted in Fig. 2.

To compare our results to those of Pagliuso et al.⁵ and Takeuchi et al.⁶ we have performed standard calculations⁵,⁶ of the magnetic susceptibility and specific heat (Fig. 3), with the splittings and wave functions from Table I as inputs. The susceptibility includes a positive molecular field contribution.
CeRhIn 5 and the wave-function mixing parameter calculation and present results obtained using the noncrossing approximation.

Comparison of the data for two different sample holders (which exhibited small differences in sample thickness and distribution) indicated similar results, augmenting our belief that the absorption correction employed is correct. If the nonmagnetic background subtraction is varied by varying \( f \) (method 1) or \( F/R \) (method 2), the scattering at 7 meV is relatively unaffected but the strength of the 24 meV scattering, and hence \( \beta \), is affected somewhat. Given the good consistency between results at different \( E_i \) and \( T \), we think that our CF scheme is basically correct. We were unable to observe QE scattering due to the requirement that to obtain the necessary resolution a small \( E_i \) is required, which causes the effects of neutron absorption (which varies as \( 1/E \)) to become large. In our fits we constrained the QE half-width to half the value of the IE width to prevent proliferation of fit parameters. Constraining to other values (e.g., \( \Gamma_{OE} = \Gamma_{IE} \)) leads only to minor variation in the final fits.

Our fits to \( \chi \) using the CF parameters plus a molecular-field term are not as good as those of Takeuchi \textit{et al.} \cite{takeuchi} or Pagliuso \textit{et al.} \cite{pagliuso} However, their fits use a value of \( \beta \) very close to unity, indicating essentially no \( \pm 3/2 \) admixture into \( |\pm 5/2\rangle \) ground state. In this case there would be no observable amplitude for the \( \Delta m_s = 1 \) transition to \( |\pm 1/2\rangle \) state at 24 meV. This cannot be correct as we clearly observe this transition in the neutron-scattering data. A possible reason that our fits are not as good as those of Refs. 5 and 6 is that we do not include the effect of exchange anisotropy, which should only be important below 20 K. Such anisotropy can be mimicked as in Pagliuso \textit{et al.} through inclusion of an anisotropic mean field parameter, which we have chosen not to do for simplicity.

On the other hand, the NCA calculations based on our CF scheme and a Kondo temperature of order 25 K does an excellent job reproducing \( \chi \). However, it overestimates the

\begin{table}
\centering
\begin{tabular}{|c|c|c|}
\hline
\( B^0_2 \) & \( B^0_4 \) & \( B^0_6 \) \\
\hline
-1.03\pm0.02 & 0.044\pm0.001 & 0.122\pm0.003 \\
\hline
\end{tabular}
\caption{Crystal-field parameters \( B^\alpha_i \), splittings and Lorentzian half-widths \( \Gamma \) of the IE excitations at four temperatures for CeRhIn 5 and the wave-function mixing parameter \( \beta \). The units of all quantities (except for \( \beta \), which is unitless) are meV. The reduced chi-square for the fit was \( \chi^2 = 0.69 \).
\end{table}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{(a) Measured anisotropic susceptibilities \( \chi^{zz} \) (triangles) and \( \chi^{zz} \) (circles) for CeRhIn 5 compared to the value calculated for the CF parameters of Table I with a molecular-field contribution \( \lambda = 35 \text{ mol/emu} \) (solid lines) and compared to the results of the NCA calculation (dashed lines). (b) Magnetic specific heat compared to the value calculated for a Schottky contribution from the excited levels and a Kondo contribution from the ground-state doublet (solid line) and to the results of the NCA calculation (dashed line).
\end{figure}

\[ \lambda = 35 \text{ mol/emu} \text{ where } \lambda \text{ represents contributions to } 1/\chi \text{ from AF and Kondo fluctuations. Thus, the calculated } \Gamma = 1/\chi_{CF} + \lambda, \text{ where } 1/\chi_{CF} \text{ is given by a standard crystal field calculation and } \lambda \text{ is chosen to provide the best fit.} \]

\[ (\Delta E_{2eV})_N = 0.003 \text{ meV, which varies as } 1/\Gamma_N. \text{ We also observe a QE contribution to } \chi \text{ at } E_i = 2 \text{ eV which is smaller than } \lambda/2. \text{ Thus, in our fits we constrained the QE half-width to half the value of the IE width to prevent proliferation of fit parameters.}

\[ \Gamma = 8 \text{ K), } \Gamma = 70 \text{ K), } \Gamma = 140 \text{ K) \\
\hline
2.3\pm0.1 & 2.9\pm0.2 & 4.2\pm0.4 \\
\hline
\end{tabular}
\caption{Comparison of the data for two different sample holders (which exhibited small differences in sample thickness and distribution) indicated similar results, augmenting our belief that the absorption correction employed is correct. If the nonmagnetic background subtraction is varied by varying \( f \) (method 1) or \( F/R \) (method 2), the scattering at 7 meV is relatively unaffected but the strength of the 24 meV scattering, and hence \( \beta \), is affected somewhat. Given the good consistency between results at different \( E_i \) and \( T \), we think that our CF scheme is basically correct. We were unable to observe QE scattering due to the requirement that to obtain the necessary resolution a small \( E_i \) is required, which causes the effects of neutron absorption (which varies as \( 1/E \)) to become large. In our fits we constrained the QE half-width to half the value of the IE width to prevent proliferation of fit parameters. Constraining to other values (e.g., \( \Gamma_{OE} = \Gamma_{IE} \)) leads only to minor variation in the final fits.

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\[ \lambda = 35 \text{ mol/emu} \text{ where } \lambda \text{ represents contributions to } 1/\chi \text{ from AF and Kondo fluctuations. Thus, the calculated } \Gamma = 1/\chi_{CF} + \lambda, \text{ where } 1/\chi_{CF} \text{ is given by a standard crystal field calculation and } \lambda \text{ is chosen to provide the best fit.} \]
width of the 7 meV excitation as seen in Fig. 2(a) and underestimates the temperature of the peak in the specific heat [Fig. 3(b)]. These deviations from the data may reflect the fact that we have neither included antiferromagnetic exchange, exchange anisotropy nor anisotropic hybridization (i.e., different hybridization to the different CF multiplets) in the NCA fits.

In summary, we find a more significant $|±3/2⟩$ admixture into $|±5/2⟩ (β=0.80)$ ground state than found earlier by Takeuchi et al.⁶ ($β=0.969$) or Pagliuso et al.⁵ ($β∼1$). The resulting CF level parameters provide reasonable fits to both the magnetic susceptibility and specific heat with the inclusion of a mean-field parameter and a Kondo doublet, respectively. In addition, NCA fits the susceptibility remarkably well with some deficiencies in both the specific heat and neutron-scattering linewidths. Taken together, the NCA calculations and the fits to specific heat and susceptibility all indicate a $T_K∼25$ K. We note that the ordered moment $gμ_B(J_z)=0.92μ_B$ deduced for $β=0.80$ is substantially larger than the value $0.37μ_B$ needed to fit the diffraction pattern in the ordered state.⁴ For our estimate of $T_K$, the moment is reduced by the Kondo physics at temperatures $T>T_N$.

We acknowledge useful discussions with W. Bao and R. J. McQueeney. Work at UC Irvine was financially supported by the UCDRD, provided by the University of California for the conduct of discretionary research by the Los Alamos National Laboratory and by the UC/LANL Personnel Assignment Program. Work at Los Alamos and Argonne was performed under the auspices of the Department of Energy. The work at Temple University was supported by the Department of Energy Grant No. DE-Fg02-01ER45827.

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