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COMMENTS AND ADDENDA

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Magnetic Resonance of Au : Er^{167} and Au : Yb^{171}

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The hyperfine splitting of (enriched) Au : Er^{167} and Au : Yb^{171} dilute alloys is reported. The absence of the signal from the $I=0$ isotopes enables a more accurate determination to be made of the hyperfine splitting parameter and of the temperature dependence of the linewidth than in a previous publication.

In a recent paper[1] (to be referred to as I) the hyperfine splittings in the magnetic-resonance spectra of dilute Au:Er and Au:Yb alloys were reported and analyzed. In measurements on the former alloy, the hyperfine splitting was completely resolved with naturally abundant isotopes. In the latter, however, the larger residual width and the small natural abundance of the $I=\frac{1}{2}$ isotope (Yb^{171}) led to an incomplete resolution of the resonance spectra requiring a superposition line-shape analysis. Because of errors possible in such an analysis (e.g., the sensitivity of the synthesized line shape and position to the assumed component resonance line shapes), we have obtained and measured the magnetic-resonance spectrum of enriched alloys.

The magnetic-resonance spectrum of Au: Er^{167} (powder sample) for an Er^{167} concentration of 100 ppm at 4.2 °K is displayed in Fig. 1(a). Figure 1(b) exhibits the magnetic-resonance spectrum of single-crystal (in an effort to reduce the residual linewidth) Au:Yb^{171} for a Yb^{171} concentration of 1000 ppm. In both cases the individual hyperfine lines possess a metallic line shape.[2] In addition, the separation of the hyperfine lines from the $I=0$ isotope line enables us to resolve the temperature dependence of their individual widths.

Using the Breit-Rabi formula, we deduce from the isotopically enriched samples that $A(\text{Au:}\,Er^{167}) = (75 \pm 0.5)$ G and $A(\text{Au:}\,Yb^{171}) = (575 \pm 10)$ G. These values are identical to those reported in I, confirming the validity of the previous analysis.

The temperature dependence of the linewidth is also close to that quoted previously.[1] For Au: Er alloys, this temperature dependence was extracted from both the $I=0$ and $I=\frac{7}{2}$ hyperfine-split lines in our current experiments. We now find, in both in-

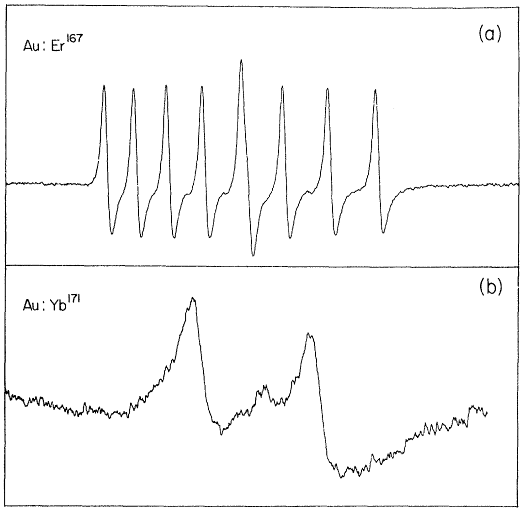

FIG. 1. (a) Electron-spin-resonance spectrum of a powdered sample of 100 ppm of Er^{167} in Au at 1.4 °K at X band. (b) Electron-spin-resonance spectrum of a single-crystal sample of 1000 ppm of Yb^{171} in Au at 1.4 °K at X band.

stances, $b(\text{Au:Er}) = (2.7 \pm 0.5)$ G/°K, rather than the value of (2.4 ± 0.2) G/°K reported previously in I (because of over-modulation effects in I). The temperature dependence of the Yb EPR linewidth was checked using the Yb^{174} ($I = 0$) enriched isotope in Au. We find $b = (40 \pm 10)$ G/°K, in agreement with the previously reported value in I. This confirmatory result is important because of the difficulties mentioned above associated with a superposition line-shape analysis, as used in I. Here use of the $I = 0$ isotope eliminates the complication of hyperfine-line overlap and enables us to determine the EPR linewidth unambiguously. A recent calculation by Barnes *et al.*[3] shows that a true hyperfine separation can obtain even in the magnetic-resonance bottleneck regime for a localized-moment exchange relaxation width less than the hyperfine splitting. However, the magnitude of the temperature-dependent linewidth would amount to only $2I/(2I+1)$ of the full local-exchange relaxation width in such a regime.

The essential identity of the temperature dependence of the previously measured $\text{Yb}(I = 0)$ line and the $\text{Yb}(I = \frac{1}{2})$ isotope linewidth presented here implies, therefore, the absence of a bottleneck in this instance. That is, if a bottleneck were present, the linewidth of the $I = 0$ isotope would bear no relation to the exchange relaxation rate of the localized moment, while for $I = \frac{1}{2}$ the linewidth of the resolved hyperfine lines would be one-half of the exchange relaxation rate. Barring a highly unlikely accident (especially in view of the concentration independence of the temperature-dependent width), equality can only mean absence of a magnetic-resonance bottleneck. This verification of the beginning assumption of I indicates their subsequent analysis to be relevant to the systems they studied.

The hyperfine constants reported in I and confirmed here were slightly larger than in nonmetallic hosts with the same local symmetry. This increase was attributed to an effective hyperfine coupling between the rare-earth effective spin and the nucleus via a dynamic polarization of the conduction electrons. The formula presented in I for this increase [Eq. (3)] is slightly in error, and should read

$$\Delta A = \left(J_{at} \frac{A_{ce}^{\text{contact}}}{g_I \mu_I} + J_{cm} \frac{A_{ce}^{cp}}{g_I \mu_I} \right) \frac{g_I \mu_I}{g_e \mu_e} \frac{\eta(E_F)}{g_J} (g_J - 1).$$

This error does not change any of the quantitative conclusions of I, with the exception that $A_{ce}^{cp}/g_I \mu_I$ is increased to -8×10^6 G. Also, a misprint in I, Eq. (1), should be corrected so that it reads

$$\Delta g = g[(g_J - 1)/g_J] J \eta(E_F).$$

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[1] L. J. Tao, D. Davidov, R. Orbach, and E. P. Chock, Phys. Rev. B 4, 5 (1971), referred to as I in the text.

[2] The A/B ratio for Au:Er^{167} is $2.5 + 0.2$, while the larger residual width and smaller intensity found for Au:Yb^{171} precludes a numerical estimate for this alloy. However, the resonance shape is suggestive of metallic character even here, as can be seen from Fig. 1(b).

[3] S. E. Barnes, J. Dupraz, and R. Orbach, J. Appl. Phys. 42, 1659 (1971).

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Calculation of Partition Functions Using the Functional-Integral Method*

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It is pointed out that if charge-density fluctuations are treated in the extremal approximation, the functional-integral method does not correctly give the thermodynamics of the Hubbard model at zero bandwidth. In particular the Schottky anomaly in the specific heat is found at one-half the exact value.

The formalism introduced by Hubbard[1] for calculating partition functions has been applied to the Anderson model[2,3] and, more recently, the Hubbard model.[4,5] These applications owe their impetus to the fact that the intra-atomic Coulomb repulsion energy $Un_\uparrow n_\downarrow$ can be written in terms of the quadratic operators $(n_\uparrow + n_\downarrow)^2$ and $(n_\uparrow - n_\downarrow)^2$; here $n_\uparrow$ and $n_\downarrow$ are fermion occupation numbers for up- and down-spin electrons, respectively. The most general way of writing $n_\uparrow n_\downarrow$ in terms of these quadratic operators is

$$n_\uparrow n_\downarrow = \alpha(n_\uparrow + n_\downarrow)^2 + (\alpha - \tfrac{1}{2})(n_\uparrow - n_\downarrow)^2 - (2\alpha - \tfrac{1}{2})(n_\uparrow + n_\downarrow), \qquad (1)$$

where α is any c number.

The most commonly chosen values for α have been $\alpha = 0$ and $\alpha = \frac{1}{4}$. The first choice, $\alpha = 0$, requires only one Gaussian field (per atomic site) in