Pressure and Temperature Dependences of $Cd_xHg_{1-x}Te$ Alloy Hall Mobilities*

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The pressure and temperature dependences of the Hall mobilities μ_H of $Cd_xHg_{1-x}Te$ alloys, with $x = 0.07$, 0.095, 0.13, and 0.18 have been measured from 4.2 to 77 °K at pressures up to 8.40 katm. The μ_H appear to be determined primarily by lattice scattering at the highest temperatures and by ionized impurity scattering at 4.2 °K. A minimum in μ_H vs T at approximately 10 °K is observed for the $x = 0.13$ and 0.18 samples. There is little variation with pressure of the temperature associated with the minimum. The variation of μ_H with energy gap E_G as determined by pressure measurements on the $x = 0.07$ and 0.13 samples is asymmetric about $E_G = 0$, in accordance with a recent theory of ionized impurity scattering in these systems which takes the variation of the dielectric constant with carrier concentration into account.

I. INTRODUCTION

This paper describes the results of measurements of the Hall coefficient R_H and Hall mobility μ_H of four samples in the system $Cd_xHg_{1-x}Te$, with x in the region 0.07–0.18. The measurements extend down to liquid-helium temperatures at pressures up to 8.4 katm. The measurements represent, to our knowledge, the first at these low temperatures and high pressures.

This particular system is of considerable technological and scientific interest because it is a mixture of a semimetal (HgTe) with a semiconductor (CdTe). The energy gap, which is defined as the $\Gamma_6 - \Gamma_8$ energy difference is negative in HgTe and $Cd_xHg_{1-x}Te$ for small x. At approximately $x = 0.16$, the system undergoes a semimetal to semiconductor transition. A considerable amount of experimental evidence has been published[1] in support of an almost linear variation of E_G with x. Since the beginning of research on the system, many attempts have been made[2–10] to analyze and explain the electrical transport properties, but few reports exist outside the $0.15 < x < 0.4$ range. These properties are understood qualitatively, for the most part, in terms of the virtual crystal approximation, in which a band structure is assumed to exist in spite of the nonperiodic nature of the alloys, and in which the band gap and effective mass vary smoothly with composition.

The performance of the research presented here is motivated by three factors. First, at low temperatures some features are observed which appear to be specific to the alloys.[10,11] Otmezguine *et al.*[11] observed a distinct minimum in μ_H versus temperature at 9 °K for samples with $x = 0.113$ and 0.129. While they attribute this anomaly to the semimetallic band structure associated with these compositions, the origin of the minimum has not yet been determined. Hence, one goal of this research was to obtain more information about the range of compositions in which the minimum occurs. In addition, it was anticipated that a knowledge of the pressure dependence would aid in its interpretation. In this work, it is shown that the minimum also appears in samples with small positive gaps, and that the position of the minimum is quite insensitive to pressure.

The second motivating factor for this research was to explore the low-temperature region in which ionized impurity scattering dominates. Here, Liu and Brust[12] suggest significant changes in the dielectric constant with carrier concentration in the small and negative band-gap region. These, in turn, according to the recent work of Gel' mont *et al.*,[13] lead to variations of μ_H with band gap, at low carrier concentrations, which are significantly different from those predicted by Long.[14] By varying the pressure, it was possible to explore the band-gap dependence of μ_H through zero band gap with the carrier concentration held relatively constant. The results tend to confirm the theory of Gel' mont *et al.*

Finally, it seemed important to systematically explore the temperature and pressure dependence of μ_H in this system because of the limited amount

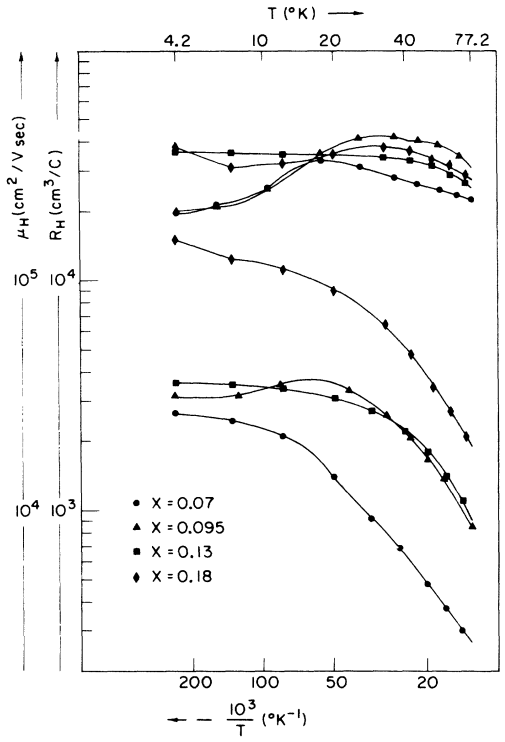

FIG. 1. Hall mobilities (upper curves) and Hall coefficients measured at 56 G in the low-temperature range on the four $Cd_xHg_{1-x}Te$ samples. Only a small number of the data points are shown to improve clarity.

of such information on small and negative gap systems.

II. EXPERIMENT

The variation of Hall coefficient and conductivity with temperature over the range 4.2–77 °K and pressure up to 8 katm has been determined experimentally for polycrystalline samples of the following alloys: $x = 0.07$, 0.095, 0.13, and 0.18. For the determination of the electrical parameters of these specimens, a sequence of systematic experiments has been performed. The samples were carefully selected. The x values of the samples have been determined using density measurements, and the homogeneity has been checked by electron microprobe analysis. This procedure assured us that the samples are homogeneous with ± 5% accuracy. However, for $x = 0.095$ and 0.18 we noticed the presence of excess mercury near the surface. For pressure measurements the samples were placed in a beryllium-copper pressure chamber with a 50% mixture of kerosene and mineral oil as the pressure-transmitting liquid. The measurements were made after subjecting the cell to a known pressure at room temperature and cooling it to 4.2 °K. The cooling was slow to ensure good hydrostatic conditions. The effect of thermal contraction on the pressure is significant only above 150 °K. Thus we may assume that in the region between 4.2–150 °K the pressure is constant. The pressure was measured by a manganin wire resistance gauge. The sample temperature was checked by a gold-iron vs copper and constantan-copper thermocouples. All measurements were carried out at $H = 56$ G. Hence, we shall discuss only those results for the transport parameters in $Hg_{1-x}Cd_xTe$ which can be derived from the conductivity and the Hall coefficient at small magnetic fields, where only the linear term of the expansion of the galvanomagnetic transport coefficient in powers of magnetic field needs to be taken into account.

To be certain that the low-field limit is appropriate, and to determine the electron and hole concentrations, measurements of the magnetic field dependence of the conductivity and Hall coefficients were made to 8 kG at 77 °K and to 32 kG at 4.2 °K. (The latter measurements were performed by Stankiewicz at Purdue University and will be described in detail in a later publication.) To determine the carrier concentrations, these data were fit with a simple two-carrier (light-electron–heavy-hole) model according to the method of Hilsum and Barrie.[15] Good fits to the data were obtained at 77 °K. At 4 °K, however, the high magnetic field data were not satisfactorily explained using the method. This failure is due, presumably, to quantum effects associated with the extremely small electron effective masses. In addition, though, equally good fits could be obtained with another model. For this reason, we cannot associate too high a degree of certainty with the carrier concentration determination. Further research on this problem is underway by Stankiewicz. The effect of this uncertainty on conclusions presented here is discussed below.

Finally, experiments were performed to show that the electrical properties measured here are not dependent on the surface treatment.

III. EXPERIMENTAL RESULTS

Curves showing the temperature dependence of the Hall coefficient R_H and mobility μ_H at atmospheric pressure for these specimens are presented in Fig. 1. R_H is negative throughout the entire temperature range down to 4.2 °K. Two features of these curves are to be noted: First, all samples show μ_H increasing with decreasing temperature down into the range of 20–40 °K, depending on the sample. At lower temperatures, the samples with $x = 0.07$ and 0.095 show μ_H decreasing with decreasing temperature. Such a behavior might be anticipated from a combination of ionized impurity (in compensated samples) and lattice scattering. The behavior of the higher-x samples is

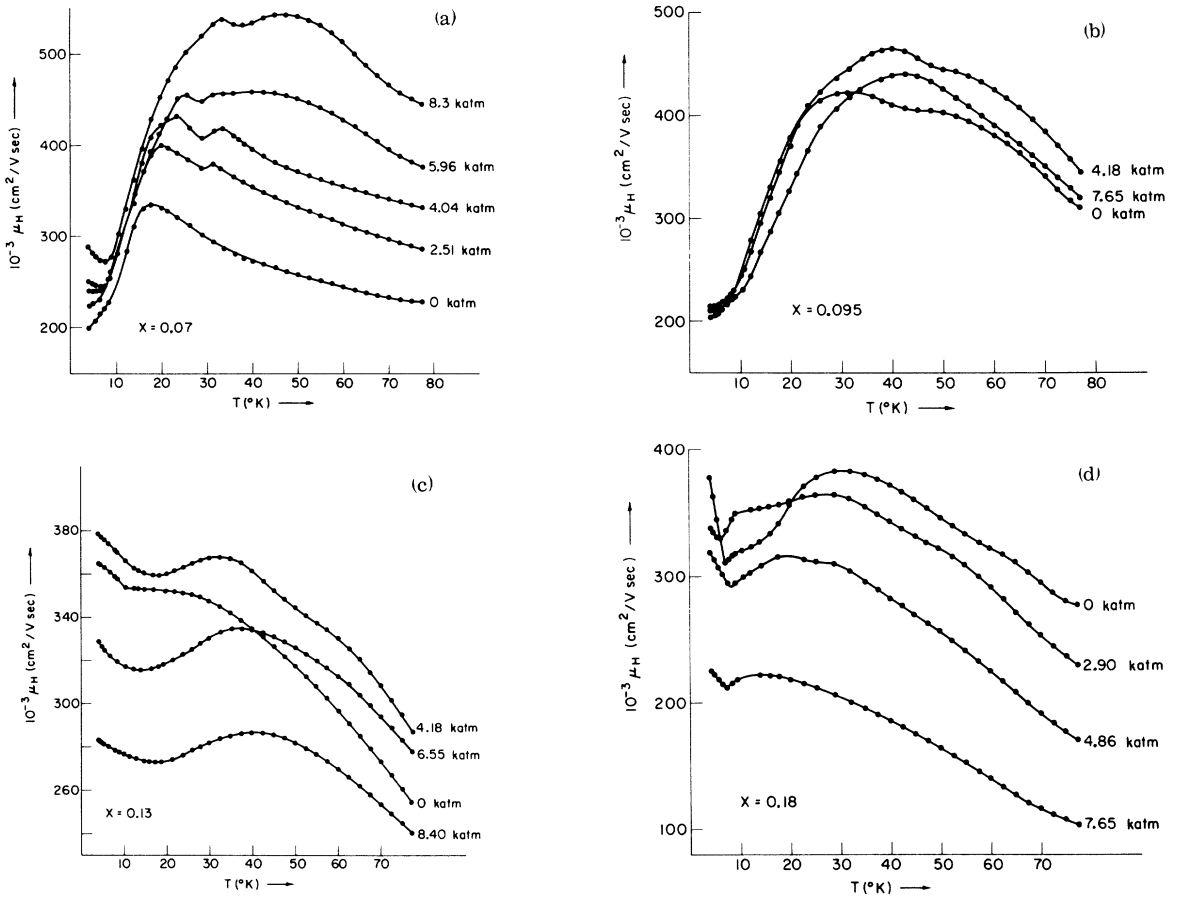

FIG. 2. (a) Hall mobilities vs temperature at various pressures for $Cd_{0.07}Hg_{0.93}Te$. (b) Hall mobilities vs temperature at various pressures for $Cd_{0.095}Hg_{0.905}Te$. (c) Hall mobilities vs temperature at various pressures for $Cd_{0.13}Hg_{0.87}Te$. (d) Hall mobilities vs temperature at various pressures for $Cd_{0.18}Hg_{0.82}Te$.

much different, however, in that the monotonic decrease of μ_H is not observed. It should be noted that the anomalous behavior of the two high-x samples is associated entirely with R_H, the conductivity varying smoothly in this region.

Figure 2(a) shows the variation of μ_H with temperature of the $x = 0.07$ sample at five different pressures. At atmospheric pressure, μ_H shows a normal increase with decreasing temperature down to approximately 19 °K, where it starts decreasing. This general behavior is typical of the five pressures at which measurements were performed, with the maximum shifting to approximately 37 °K at 8.3 katm. All the elevated-pressure measurements show, in addition, however, a subsidiary minimum between 30 and 40 °K. For $T > 30$ °K, the mobility increases monotonically with increasing pressure, at constant temperature. Finally, at the highest pressure, the mobility shows another minimum below 10 °K. The increase at temperatures below the minimum amounts to less than 5% of μ_H at the minimum, so that the existence of the minimum cannot be considered too reliable.

Figure 2(b) shows similar curves for the $x = 0.095$ sample. Again, the general form is the expected increasing μ_H with decreasing T at high T, followed by a decrease. The maxima shift to a higher temperature relative to the $x = 0.07$ sample. In addition, there are subsidiary minima at atmospheric and 4.18 katm pressures in the region between 40 and 50 °K. This minimum is not apparent in the 7.65-katm data. It should also be noted that there is no trace of the minimum below 10 °K in these data. Finally, it should be noted that μ_H is not a monotonically increasing function of pressure for this sample at high T. μ_H increases in going from 0 to 6.4 katm. (see Fig. 3) and then decreases in going from 6.4 to 7.65 katm.

Figure 2(c) depicts the variation for the $x = 0.13$ sample. Superimposed on the previously discussed temperature dependences is a cusp in the atmospheric-pressure data at 10 °K. With the increasing pressure, the cusp becomes a soft minimum between 14 and 18 °K, depending on the pressure.

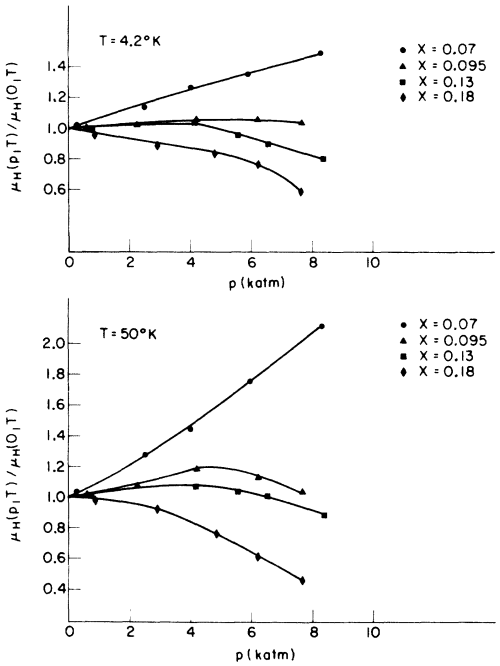

FIG. 3. Dependence of the Hall mobility on pressure for $Cd_xHg_{1-x}Te$ samples at the temperatures 4.2 and 50 °K.

Again, at high T, μ_H increases between 0 and 4.18 katm and then decreases between 4.18 and 8.40 katm.

Figure 2(d) presents the data for the $x = 0.18$ sample. This sample differs from that with $x = 0.13$ in that the low-temperature minimum becomes extremely sharp and falls between 7 and 9 °K at all pressures. In addition, the high-temperature μ_H decreases with increasing pressure.

The change of the Fermi level E_F with pressure at 4.2 °K in these samples was calculated using the expression relating E_F to the carrier concentration E_G and m^* derived by Harman and Honig.[16] In these calculations, the E_G and their pressure dependences were taken from the work of Stankiewicz and Giriat[17] and the assumption that the pressure dependences are the same at 4.2 as at 77 °K and that the linear dependence of E_G on temperature extends down to 4.2 °K. While there must be curvature in E_G vs T at very low T, this has not yet been observed and should not lead to any significant modifications of the parameters. The pressure dependences, carrier concentrations, E_G, and E_F are presented as a function of P in Table I.

IV. DISCUSSION

In this section we shall attempt to explain many of the features of the observed pressure and temperature dependences of μ_H. Sections IV A and IV B deal with properties which are readily understood in a qualitative manner through the pressure and temperature dependences of the band parameters and scattering mechanisms. Section IV C deals

TABLE I. Variation of E_F with pressure, as well as parameters used in calculating them (matrix element $P = 8.3 \times 10^{-8}$ eV cm).

x	$\frac{dE_G}{dp}$ (meV/katm)	P (katm)	$n = \frac{1}{ecR_H}$ (cm^{-3})	E_G (meV)	E_F (meV)
0.07	9.5	0	2.35×10^{15}	−170	4.4
		2.51	1.84×10^{15}	−146	4.4
		4.04	1.55×10^{15}	−132	4.4
		5.96	1.42×10^{15}	−113	4.7
		8.30	1.40×10^{15}	−91	5.7
0.095	10.5	0	1.97×10^{15}	−120	5.5
		2.27	1.84×10^{15}	−96	6.3
		4.18	1.73×10^{15}	−76	7.6
		6.20	1.62×10^{15}	−55	9.4
		7.65	1.54×10^{15}	−40	11.5
0.13	9.6	0	1.73×10^{15}	−60	9.2
		0.75	1.66×10^{15}	−53	9.8
		4.18	1.46×10^{15}	−20	15.8
		5.55	1.46×10^{15}	−7	20.6
		6.55	1.46×10^{15}	3	22.4
		8.40	1.52×10^{15}	21	15.9
0.18	8.5	0	4.16×10^{14}	20	8.6
		0.85	3.92×10^{14}	27	6.9
		2.90	3.50×10^{14}	45	4.5
		4.86	3.02×10^{14}	61	3.1
		6.20	2.66×10^{14}	73	2.4
		7.65	2.66×10^{14}	85	2.1

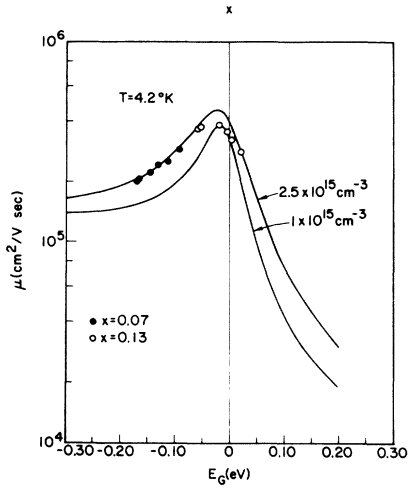

FIG. 4. Ionized impurity scattering mobility vs energy gap in $Cd_xHg_{1-x}Te$ at 4.2 °K. The curves are theoretical while the points show experimental data for the $x = 0.07$ and 0.13 samples. The data points are from samples having carrier concentrations in the range (1–2.5) $\times 10^{15}$ cm^{-3}. The curves were calculated for $2N_A = 11.5 \times 10^{15}$ cm^{-3}.

with properties which we understand very much less well.

A. High-Temperature Mobility Pressure Dependence

The pressures dependences of μ_H at 4 and 50 °K for the four samples are shown in Fig. 3. It should be noted, first of all, that the pressure dependences are much stronger at 50 than at 4 °K. We interpret this as being due to the predominance of lattice scattering at high T and ionized impurity scattering at low T, with the corresponding strong and weak dependences on the electron effective mass. At 50 °K, then, the predominant effect of pressure is to alter the electronic effective mass. For the $x = 0.18$ sample, Γ_6 lies above Γ_8 (positive energy gap) and the gap increases with increasing pressure. Consequently, m^* increases and μ_H decreases with increasing P. In the $x = 0.07$ sample, on the other hand, Γ_6 lies below Γ_8, so that the conduction band is the light-mass Γ_8 band. As P increases, the magnitude of the negative gap decreases, so that the conduction-band mass decreases and the mobility increases with increasing P.

In the $x = 0.095$ and 0.13 samples at 50 °K, the gap is negative at atmospheric pressure. With increasing pressure, however, the gap reverses sign. Consequently, m^* decreases with increasing pressure until the gap closes, and then increases with increasing pressure. As a result, the mobilities show maxima with increasing pressure. Since the pressure and temperature dependences of the energy-band parameters have been determined previously from similar measurements[17] at 77 °K, the results will not be discussed in greater detail.

B. 4 °K Mobility Pressure Dependences

At 4 °K, it is anticipated that ionized impurity scattering dominates μ_H^{-1}. Of particular interest here is the variation of μ_H as the band gap changes from negative to positive. Long[14] has calculated the dependence of μ_H on both E_G and carrier concentration, taking nonparabolicity into account and assuming that the dielectric constant is a smoothly varying function of x. He finds, at fixed carrier concentrations, that μ_H vs E_G shows a sharply peaked symmetric maximum at $E_G = 0$. Gel'mont *et al.*[13] also have taken explicitly into account, in addition, the dependence of the dielectric constant on carrier concentration proposed by Liu and Brust.[12] This effect is appreciable for negative E_G and breaks the symmetry around $E_G = 0$. The breaking of the symmetry at 77 °K, in samples with $x = 0.113$ and 0.107 has been found experimentally by Otmezguine *et al.*[11] In this work, the symmetry breaking is shown at 4.2 °K and compared with the Gel'mont *et al.* theory.

The pressure dependence of μ_H at 4.2 °K of the $x = 0.13$ sample provides a good test of the two theories, since E_G changes from negative to positive with application of pressure. The results are listed in Table I and shown in Fig. 4 (open circles). From Fig. 4, it can be seen that there is a very small increase in mobility as E_G approaches zero from the negative side and then a sharp decrease in the mobility as E_G goes through zero and becomes increasingly positive. To convert from pressure to E_G for each sample, the data of Stankiewicz and Giriat[17] were used.

The observation of such an asymmetry depends sensitively, though, on the determination of the pressure which corresponds to $E_G = 0$. For this reason, we have attempted to determine a maximum uncertainty in that pressure. In Fig. 4 and Table I, we have used a zero-pressure gap of -60 meV and a pressure dependence given by $dE_G/dp = 9.6$ meV/katm.[17] With these parameters, $E_G = 0$ corresponds to $p = 6.25$ katm. The results could be made to appear more symmetric if a lower pressure were associated with $E_G = 0$. To obtain a lower limit on that pressure, a lower limit on the zero-pressure magnitude of E_G and an upper limit on dE_G/dp must be obtained. The smallest E_G we have seen predicted for a sample of this composition is given by the empirical equation of Schmit and Stelzer[18] extrapolated into this composition range. This value is $E_G = -41$ meV. To give the reader some idea of the uncertainties involved in extrapolating these empirical equations, we should point out that the equation of Scott[19] yields -76 meV. Similarly, from the results presented by Stankiewicz and Giriat[17] and by Otmezguine *et al.*,[11] we

believe an upper bound on dE_G/dp is 10.5 meV/katm. Using these numbers, the $E_G = 0$ vertical line on Fig. 4 would be shifted to the abscissa value now denoted as $E_G = -25$ meV. In this case, the maximum measured mobility would be close to this new zero-gap position. Nevertheless, the asymmetry is still apparent, since there is very little decrease of μ_H for decreasing negative E_G relative to the decrease for increasing positive E_G.

By fortunate coincidence, the $x = 0.07$ sample has the same computed N_A as the $x = 0.13$ sample. Hence, it was possible to compare data from both samples on the same curve with the theoretical calculations discussed immediately below. The previously mentioned concern about ambiguities in the determination of the carrier concentrations should be recalled, however.

Finally, Fig. 4 shows the results of recalculations of μ_H vs E_G, based on the theory of Gel'mont *et al.*,[13] for the compensated samples with $2N_A = 11.5 \times 10^{15}$ cm^{-3} used here. As can be seen the asymmetry is quite evident in the calculated curves and the agreement between theory and experiment is quite reasonable. Again, though, we must caution the reader to recall the uncertainties in the carrier concentration determination and must also point out that the carrier concentration itself could change markedly with pressure as the gap changes from negative to positive. Hence, while the agreement between theory and experiment is good, these results cannot yet be taken as a very strong confirmation of the theory.

C. Low-Temperature Minimum in μ_H

We have not been able, as a result of this work, to provide a mechanism for the low-temperature minima in the $x = 0.13$ and 0.18 samples. Some features are worth noting, however:

First it should be observed that the minima are typical of the positive band-gap studies here. Hence, the phenomenon is not tied directly to the existence of a negative energy gap.

Another interesting feature of these measurements is the insensitivity of the temperature associated with the minimum to pressure. This is particularly true of the $x = 0.18$ sample, in which the gap is varied from 20 to 85 meV, while the temperature varies by less than 2 °K. The temperature variation in the $x = 0.13$ sample is not much larger.

The most important aspect of the work presented thus far is, however, the fact that the theory of Gel'mont *et al.*, appears to apply at 4.2 °K, which is below the temperature of the minimum. Hence, if the theory is truly applicable, it should be able to predict the minimum. Unfortunately, no calculations of the temperature dependence of μ_H based on this theory have been performed thus far. These are now underway, however.

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