Padé Approximant Bounds for the Magnetic Susceptibility in the Three-Dimensional, Spin-$\frac{1}{2}$ Heisenberg Model*

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We show that the analytical properties of a function and the first few terms of its power series may be utilized to obtain upper and lower bounds for a function and its derivative. We apply this technique to the Heisenberg-model susceptibility series and show that they diverge like $(1-T/T_c)^{-\gamma}$ at the Curie point, where γ is very closely $\frac{4}{3}$. Fairly accurate values of the Curie point are given for three lattices.

INTRODUCTION

At the present time a defect of the Padé approximant method[1] is that, although it converges rapidly, accurate estimates of its error are not available. In this paper we show that if certain transformations are applied to the perturbation series then it is possible to obtain upper and lower bounds to the function and its derivative. We apply these results to the magnetic susceptibility of the three-dimensional spin-$\frac{1}{2}$ Heisenberg model. We are able to establish with an error of at most 0.01 for the body-centered and face-centered cubic lattice that the susceptibility behaves as $(1-T_c/T)^{-4/3}$ near the Curie point. Fairly accurate estimates for the critical temperatures are given for the simple cubic, body-centered cubic, and face-centered cubic lattices.

II. REDUCTION OF BOUNDED ANALYTIC FUNCTIONS TO STIELTJES SERIES

By and large there are two main types of questions which physicists seek to answer from perturbation theory calculations. The first is the value of some real function at a real point. If the perturbation series converges, then the results of this section provide a method of obtaining (rapidly) converging upper and lower bounds for the answer. In addition these results are available for certain types of asymptotic series. The second type of question is the location of some real singularity of physical significance in a real function, e.g., the critical point for a thermodynamic system. The results here are frequently sufficient to provide bounds on the location of the singularity, and some bounds on quantitative properties of the function in the neighborhood of the singular point.

The first step is to transform functions which are bounded from below into Stieltjes series. Any series which can be formally written in the form

$$F(t)=\sum_{j=0}^{\infty} f_j(-t)^j=\int_0^m \frac{d\varphi(u)}{1+ut}, \tag{2.1}$$

is called a Stieltjes series. The weight function φ is assumed to be monotonic nondecreasing and m may be infinite. Necessary and sufficient conditions[2] for form (2.1) to hold are that

$$\begin{aligned} &D(0,n)>0, \quad n=0,1,\cdots,\\ &D(1,n)>0, \quad n=0,1,\cdots, \end{aligned} \tag{2.2}$$

where

$$D(m,n)=\det\begin{vmatrix} f_m & f_{m+1} & \cdots & f_{m+n}\\ \vdots & \vdots & \ddots & \vdots \\ f_{m+n} & f_{m+n+1} & \cdots & f_{m+2n}\end{vmatrix}. \tag{2.3}$$

We now introduce the $[M,N]$ Padé approximants. The $[M,N]$ Padé approximant to a function $F(t)$ is defined by the equations

$$\begin{aligned} F(t)Q_M(t)-P_N(t)&=O(t^{M+N+1}),\\ Q_M(0)&=1.0,\\ [M,N]&=P_N(t)/Q_M(t), \end{aligned} \tag{2.4}$$

where Q_M and P_N are polynomials of degree M and N, respectively. For Stieltjes series and t real and positive they have the properties[2]

$$(-1)^{1+j}\{[N+1,N+1+j]-[N,N+j]\}\geq 0, \tag{2.5a}$$

$$(-1)^{1+j}\{[N,N+j]-[N-1,N+j+1]\}\geq 0, \tag{2.5b}$$

$$[N,N]\geq F(t)\geq [N,N-1], \tag{2.5c}$$

$$[N,N]'\geq F'(t)\geq [N,N-1]', \tag{2.5d}$$

for $j\geq -1$. These inequalities have the consequence that the $[N,N]$ and $[N,N-1]$ form the best obtainable Padé approximant upper and lower bounds from a given number of coefficients and that the use of additional coefficient improves the bounds. $[N,N]'$ converges monotonically from above, $[N,N-1]'$ need not converge monotonically, but is the best lower Padé bound obtainable for the derivative $F'(t)$.

To transform a function bounded from below into a

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[1] See, for example, G. A. Baker, Jr., J. L. Gammel, and J. G. Wills, J. Math. Anal. Appl. 2, 21, 405 (1961); G. A. Baker, Jr., Phys. Rev. 124, 768 (1961); 129, 99 (1963).

[2] T. J. Stieltjes, Ann. Fac. Sci. Toulouse 8, 1 (1894); 9, 1 (1894). A more recent reference is H. S. Wall, *Analytic Theory of Continued Fractions* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1948). See also, G. A. Baker, Jr., Advan. Theoret. Phys. (to be published) for a thorough review of the relevant theory from a physicist's point of view.

series of Stieltjes we need the following theorem due to Riesz[3] and Herglotz.[4]

The most general expression for an analytic function $f(z)$ which is regular and has a positive real part for $|z|<1$, and which is real for real values of z, is

$$f(z)=\frac{1+z}{1-z}\int_0^{2\pi}\frac{d\varphi(t)}{1+[4z/(1-z)^2]\sin^2(\frac{1}{2}t)}, \quad (2.6)$$

where φ is monotonic nondecreasing.

Proof: Suppose $f(z)$ is regular inside $|z|<1$, then if we pick for a contour a circle of radius $r<1$, then if $|z|<r$, we have by Cauchy's theorem

$$f(z)=\frac{1}{2\pi i}\oint\frac{f(w)dw}{w-z}, \qquad f^{(n)}(0)/n!=\frac{1}{2\pi i}\oint f(w)w^{-1-n}dw. \quad (2.7)$$

If $w=re^{i\theta}$ and $f(re^{i\theta})=h(\theta)+ig(\theta)$, then (2.7) becomes

$$f^{(n)}(0)/n!=\frac{r^{-n}}{2\pi}\int_{-\pi}^{\pi}[h(\theta)\cos n\theta+g(\theta)\sin n\theta]d\theta, \quad (2.8)$$

as $f^{(n)}$ is assumed real. We note that for n negative the integral in (2.8) vanishes, so if we multiply the $-n$ case by r^{-2n} and add it to (2.8) we get

$$f(0)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}h(\theta)d\theta, \quad f^{(n)}(0)/n!=\frac{r^{-n}}{\pi}\times\int_{-\pi}^{+\pi}h(\theta)\cos n\theta d\theta, \quad n\geq 1. \quad (2.9)$$

However, by assumption $h(\theta)>0$. Thus, if we define

$$\varphi(t)=\lim_{r\to 1}\frac{1}{\pi}\int_{-\pi}^{t}h(\theta)d\theta, \quad (2.10)$$

it will be monotonic nondecreasing, and if we multiply (2.9) by z^n and sum over $n=0$ to ∞ we obtain

$$\begin{aligned}f(z)&=\tfrac{1}{2}\int_{-\pi}^{+\pi}[1+2\sum_{n=1}^{\infty}(\cos nt)z^n]d\varphi(t)\\&=\int_{-\pi}^{+\pi}\frac{1-z^2}{1-2z\cos t+z^2}d\varphi(t)\\&=\frac{1+z}{1-z}\int_{-\pi}^{\pi}\frac{d\varphi(t)}{1+[4z/(1-z)^2]\sin^2(\frac{1}{2}t)}, \quad (2.11)\end{aligned}$$

which completes the proof.

Suppose now we have a function $f(z)$ which is regular for $|z|<1$, and bounded from below there. We may, therefore, add a constant M to give it a positive real part. Let us further make the change of variables

$$z=[(1+w)^{1/2}-1]/[(1+w)^{1/2}+1]; \quad (2.12)$$

then, by the Riesz-Herglotz theorem, we find

$$F(w)\equiv\{f([(1+w)^{1/2}-1]/[(1+w)^{1/2}+1])+M\}\times(1+w)^{-1/2}=\int_{-\pi}^{+\pi}\frac{d\varphi(t)}{1+w\sin^2(\frac{1}{2}t)}. \quad (2.13)$$

If we use $\sin^2(\frac{1}{2}t)$ as a variable, then (2.13) implies (2.1) with an upper limit of 1 which in turn implies that for any $f(z)+M$ satisfying the conditions of the Riesz-Herglotz theorem, $F(w)$ is a series of Stieltjes with radius of convergence of at least unity. The transformation (2.12) has the effect of mapping the interior of the unit circle in the z plane onto the cut w plane $(-\infty,-1)$. The coefficients of $F(w)$ are readily given in terms of those of $f(z)$ by the following formula due to Gronwall[5]:

$$f(z)=\sum_{j=0}^{\infty}f_j(-z)^j, \quad F(w)=\sum_{j=0}^{\infty}F_j(-w)^j, \qquad F_j=4^{-j}\sum_{k=0}^{j}\binom{2j}{j-k}(f_k+\delta_{k,0}M), \quad (2.14)$$

where $\delta_{k,0}$ is the Kronecker delta function.

If we now form $[N,N+j]$ Padé approximants to $F(w)$, then by the properties (2.5) for w real and positive, the j even approximants and their derivatives all lie above the correct value and the j odd approximants and their derivatives all lie below the correct value. Convergence from above and below is assured[2] and it is monotonic in N (exception: $[N,N-1]$ slope which is even so a better lower bound than any other odd j slope).

We will now expand the class of real functions to which these results are applicable. Suppose that there is a branch point at $0<+R_1<1$ and another one at $-1<R_2<0$. Let us distort the contour of the proof of the Riesz-Herglotz theorem to run as follows: Begin at R_1, procede along the real axis (branch of function continued from upper half-plane) to $+r<1$, continue in upper half-plane along arc $|z|=r$ to $z=-r$, then along negative real axis to $z=-R_2$ (branch of function continued from upper half-plane), and close the contour by following the complex conjugate path to the one just described. Now since $f(z)$ is a real function for real z, it follows from Schwarz's principle of symmetry[6] that the discontinuity across the cuts is purely imaginary as

[3] F. Riesz, Ann. École Normale 28, 34 (1911).
[4] G. Herglotz, Leipzig Ber. 63, 501 (1911).

[5] T. H. Gronwall, Ann. Math. 33, 101 (1932).
[6] See, for example, E. T. Copson, *An Introduction to the Theory of Functions of a Complex Variable* (Oxford University Press, London, 1948), Sec. 8.4.

$f(\rho+i\epsilon)=f^*(\rho-i\epsilon)$. Equation (2.9) becomes

$$f(0)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}h(\theta)d\theta+\frac{1}{\pi}\int_{-r}^{-R_2}\mathrm{Im}[f(\rho+i\epsilon)]\times\frac{d\rho}{\rho}+\frac{1}{\pi}\int_{R_1}^{r}\mathrm{Im}[f(\rho+i\epsilon)]\frac{d\rho}{\rho},$$

$$f^{(n)}(0)/n!=\frac{r^{-n}}{\pi}\int_{-\pi}^{+\pi}h(\theta)\cos n\theta d\theta \tag{2.15}$$
$$+\frac{1}{\pi}\int_{-r}^{-R_2}\mathrm{Im}[f(\rho+i\epsilon)][\rho^{-1-n}+\rho^{n-1}r^{-2n}]d\rho$$
$$+\frac{1}{\pi}\int_{R_1}^{r}\mathrm{Im}[f(\rho+i\epsilon)]\times[\rho^{-1-n}+\rho^{n-1}r^{-2n}]d\rho\quad n\geq 1.$$

If we multiply (2.15) by z^n and sum, we get

$$f(z)=\frac{1+z}{1-z}\int_{-\pi}^{+\pi}\frac{d\varphi(t)}{1+[4z/(1-z)^2]\sin^2(\frac{1}{2}t)}+\frac{1}{\pi}\frac{(1+z)}{(1-z)}\times\int_{-1}^{-R_2}\frac{\rho^{-1}\,\mathrm{Im}[f(\rho+i\epsilon)]d\rho}{1-[(1-\rho)^2/4\rho][4z/(1-z)^2]}+\frac{1}{\pi}\frac{(1+z)}{(1-z)}\times\int_{R_1}^{1}\frac{\rho^{-1}\,\mathrm{Im}[f(\rho+i\epsilon)]d\rho}{1-[(1-\rho)^2/4\rho][4z/(1-z)^2]} \tag{2.16}$$
$$=\frac{1+z}{1-z}\int_{-T_1}^{T_2}\frac{d\Phi(T)}{1+[4z/(1-z)^2]T},$$

$$T_1=\tfrac{1}{4}(1-R_1)^2/R_1,\quad T_2=\tfrac{1}{4}(1+R_2)^2/R_2,$$

where $\Phi(T)$ is defined by combining the other three integrals. $\Phi(T)$ defined this way will be monotonic nondecreasing if and only if $\rho^{-1}\,\mathrm{Im}[f(\rho+i\epsilon)]\geq 0$ and $h(\theta)>0$. If we define $F(w)$ from $f(z)$ as in (2.13), then it follows that

$$\hat{F}(u)=(1+T_1u)^{-1}F[u(1+T_1u)^{-1}] \tag{2.17}$$

is a series of Stieltjes which is regular in the cut u plane $[-\infty,-(T_1+T_2)^{-1}]$. From theorem 1 of Baker, Gammel, and Wills,[1] we note that the $[N,N]$ approximants have all the various properties in the cut plane $(-\infty,-T_2^{-1})$, $(T_1^{-1},+\infty)$.

We see from form (2.16) that we may, with impunity, let $R_2\rightarrow 0$ $(T_2\rightarrow+\infty)$ and retain $\hat{F}(u)$ as a series of Stieltjes. We have now proved the following theorem:

Let $f(z)$ be a function possessing all real right-hand derivatives of $z=0$. Let $f(z)$ be analytic $|z|<1$, $\mathrm{Im}(z)\neq 0$, and $\mathrm{Re}f(z)$ bounded from below by a constant $-M$ there. Further, let $f(z)$ be such that $\lim_{\epsilon\rightarrow 0^+}\times x^{-1}f(x+i\epsilon)\geq 0$ for real $-1<x<+1$. Then $\hat{F}(u)$ is a Stieltjes series where

$$\hat{F}(u)=(1+T_1u)F(u(1+T_1u)^{-1}),$$
$$F(w)=\{f([(1+w)^{1/2}-1]/[(1+w)^{1/2}+1])+M\}\times(1+w)^{-1/2}, \tag{2.18}$$
$$T_1=\tfrac{1}{4}(1-R_1)^2/R_1,$$

where R_1 is the minimum of 1 and the least upper bound of real regular points of f (which bound we assume to be positive). Convergent bounds to $f(z)$ are then given via $\hat{F}(u)$ by properties (2.5).

A couple of examples will suffice to indicate the nature of the requirement on the imaginary part. Basically it means that the type of singularity which is acceptable is one which vanishes for x positive no faster than linearly and diverges for x negative no faster than linearly. Functions such as

$$A-z/\ln(\beta-z),\qquad 0<\beta<1,$$
$$A+(\beta-z)^\alpha,\qquad 2N\leq\alpha\leq 2N+1,$$

where N is an integer (positive negative, or zero) are allowed. For z negative,

$$A+(\beta+z)^\alpha,\quad 2N-1\leq\alpha\leq 2N$$

is, for example, allowed. A few simple manipulations using some physical knowledge frequently suffice to cast a function with a physical singularity into manageable form.

In case the region in which the conditions of our theorem are satisfied is not the unit circle, we know by Riemann's theorem on conformal mapping[7] that we can analytically map any simply connected domain with a reasonable boundary curve into the unit circle. If the other domain is a circle, then a linear fractional transformation is a very convenient one to use.

III. MAGNETIC SUSCEPTIBILITY FOR THE HEISENBERG MODEL ON SOME THREE-DIMENSIONAL LATTICES

At present, the following coefficients in the series expansion of the reduced spin-$\frac{1}{2}$ Heisenberg-model magnetic susceptibility are known.[8]

$$\chi_{sc}=1+3K+6K^2+11K^3+\frac{165}{8}K^4+\frac{1561}{40}K^5+\frac{33\,013}{480}K^6+\frac{100\,321}{840}K^7+\frac{968\,407}{4480}K^8+\cdots, \tag{3.1a}$$

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[7] See, for example, C. Carathéodory, *Conformal Representation* (Cambridge University Press, New York, 1932), Chap. V.

[8] C. Domb, Phil. Mag. Suppl. **9**, 149 (1960); C. Domb and D. W. Wood, Phys. Letters **8**, 20 (1964).

$$\chi_{\mathrm{bcc}}=1+4K+12K^2+\frac{104}{3}K^3+\frac{575}{6}K^4+\frac{2627}{10}K^5+\frac{16\,993}{24}K^6+\frac{4\,771\,090}{2520}K^7+\frac{3\,368\,137}{672}K^8+\cdots, \quad (3.1\mathrm{b})$$

$$\chi_{\mathrm{fcc}}=1+6K+30K^2+138K^3+\frac{2445}{4}K^4+\frac{53\,171}{20}K^5+\frac{914\,601}{80}K^6+\cdots, \quad (3.1\mathrm{c})$$

where $K=J/(2kT)$, J=exchange integral, and sc stands for simple cubic lattice, bcc, for body-centered cubic lattice, and fcc, for face-centered cubic lattice.

Our procedure for extracting relevant information from them is as follows. First, for some function $f(z)$ (related to χ), we hypothesize that in and on a circle with diameter $(-a, b)$, $f(z)+A$ is in the class of functions described just before Eq. (2.15). Second, we map that circle onto the unit circle so that

$$g(z)=f\left(\frac{2z}{(a^{-1}+b^{-1})-(a^{-1}-b^{-1})z}\right)+A \quad (3.2)$$

is of a form to which we may apply the theorems of the previous section. It then follows that

$$h(w)=g\left[\frac{(1+w)^{1/2}-1}{(1+w)^{1/2}+1}\right](1+w)^{-1/2} \quad (3.3)$$

is of the form

$$h(w)=\int_{-T_1}^{T_2}\frac{d\Phi(T)}{1+wT}, \quad (3.4)$$

where $\Phi(T)$ is monotonic nondecreasing. In practice, we will make our hypotheses in such a way that $T_1=0$. The coefficients for h are given in terms of those for g by (2.14). We then compute the approximation to $f(x)$ as

$$\{(1+w)^{1/2}[N,M](w)-A\}, \quad (3.5)$$

where

$$w=\frac{2(a^{-1}+b^{-1})x[1+\frac{1}{2}(a^{-1}-b^{-1})x]}{[1-b^{-1}x]^2}. \quad (3.6)$$

The properties of upper and lower bounds to the function are preserved, as are those for the slopes. For the slope one must check the values of the slope of the approximants in order to tell whether the slope at an unknown but bounded point is bounded by the slope at the upper or lower bound.

In order to investigate the nature of the Curie point singularity in the reduced susceptibility and to compare it with earlier estimates by Domb and Sykes[9] and Baker[10] we have first considered $[d\ln\chi/dK]^{-1}$ for the close-packed face-centered cubic lattice and $[1+Kd\ln\chi/dK]^{-1}$ for the loose-packed body-centered cubic and simple cubic lattices. The reason for these choices is as follows: If χ has, as is believed, a singularity like $(K_c-K)^{-\gamma}$, then the reciprocal of the logarithmic derivative has a zero with slope $-\gamma^{-1}$ at K_c. For the loose-packed lattices, if the behavior at antiferromagnetic Curie point is anything like that found by Fisher and Sykes[11] for the Ising model, then $[d\ln\chi/dK]^{-1}$ will have a discontinuity in the imaginary part of the wrong sign, but $[1+Kd\ln\chi/dK]^{-1}$ will not. Our best results from this analysis [via (2.5)] are given in Table I.

TABLE I. Analysis of $d\ln\chi/dK$.

	K_c		Slope at K_c				
Lattice	Lower bound	Upper bound	Upper bound	Lower bound	a	b	A
sc	0.587035	0.624236	−0.945259	−2.65147	0.5	2.0	4.0
bcc	0.391797	0.397654	−1.24217	−1.55727	0.5	1.5	2.5
fcc	0.245919	0.246945	−1.31287	−1.36295	1.0	0.8	0.6

The best results are for the face-centered cubic lattice. These strongly suggest $\gamma=\frac{4}{3}$, in agreement with Domb and Sykes.[9] The bounds for the other lattices are consistent with this value. We have computed $\chi^{-3/4}$ which should, if $\gamma=\frac{4}{3}$ is correct, have a zero at K_c. Our results from this analysis [via (2.5)] are given in Table II. There are values of K_c which satisfy the requirements of both Tables I and II. We adopt as the most likely values of K_c

$$\begin{aligned}&\mathrm{sc} && K_c=0.588,\\ &\mathrm{bcc} && K_c=0.3923,\\ &\mathrm{fcc} && K_c=0.2460,\end{aligned} \quad (3.7)$$

TABLE II. K_c from analysis of $\chi^{-3/4}$.

Lattice	Lower bound	Upper bound	a	b	A
sc	0.574203	0.588134	0.5	2.0	2.0
bcc	0.392045	0.392313	0.5	1.5	1.5
fcc	0.245601	0.246042	1.0	0.8	4.0

where the last figure must be considered uncertain. As a check on the hypothesis that $\gamma=\frac{4}{3}$, we have computed, using Padé approximants, $(K_c-K)(d\ln\chi/dK)$ at $K=K_c$. This value should be $\frac{4}{3}$ if the hypothesis is correct. We list our results in Table III. We consider

TABLE III. γ from $(K_c-K)(d\ln\chi/dK)$.

Lattice	Lower bound	Upper bound	a	b	A
sc	1.254	1.347	0.5	2.0	4.0
bcc	1.326	1.343	0.5	1.5	1.0
fcc	1.332	1.337	1.0	0.8	2.0

[9] C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).

[10] G. A. Baker, Jr., Phys. Rev. **129**, 99 (1963).

[11] M. E. Fisher and M. F. Sykes, Physica **28**, 919, 939 (1962).

them to be good confirmation, at least for the body-centered cubic and face-centered cubic lattice. The series for the simple cubic lattice seems to be more irregular and the results converge more slowly, but we know of no reason why it should be qualitatively different from the body-centered cubic.

Our results depend on the hypotheses we have made concerning the nature of the functions studied. We detect no violation of the hypotheses, but, of course, we cannot prove them either. The results we obtain agree very well with those of Rushbrooke and Wood[12] for the bcc and sc and those of Domb and Sykes[9] for the fcc.

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Heat Capacity of Ordered and Disordered CuPt Below 4.2°K

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Heat-capacity measurements below 4.2°K on CuPt show that the electronic heat-capacity coefficient γ decreases from 0.825 mJ mole^{-1} deg^{-2} in the disordered condition to 0.530 in the ordered condition. The Debye temperature increases on ordering from 357 to 385°K. It is suggested that the observed changes can be explained either in terms of the alterations in the Brillouin zone structure which occur on ordering or by the possibility of a magnetic transition in the ordered condition.

The order-disorder transformation in the CuPt system which occurs in the alloy of 50 at.% is unusual, since the number of unlike nearest neighbors in the ordered condition is the same as it is, on the average, in the random disordered condition.[1] Consequently, an explanation of the tendency toward ordering which is based on a decreased interaction energy for unlike nearest neighbors (quasichemical theory) is not applicable.

The effect of superlattice formation on the Brillouin zone structure of an alloy has been discussed by several authors.[2–5] When a superlattice forms in an alloy, the x-ray structure factor for certain planes is no longer equal to zero, as it is in the disordered condition. These extra superlattice reflections give rise to a reduction in the size of the basic Brillouin zone, which can lower the electronic energy of the alloy by interacting with the electrons near the Fermi surface. Since all of the electrons in the alloy partake of this interaction and since its existence does not require that the number of unlike nearest neighbors change, it is an attractive explanation for the tendency toward ordering in CuPt and has been elaborated upon in further detail by Nicholas.[6] Although it is difficult to predict in detail what effects the Brillouin zone–Fermi surface interface due to superlattice formation should have on the electronic structure, it is possible that the density of states curve could be changed. An earlier investigation of the low-temperature heat capacity of Cu_3Au[7] showed no difference in the electronic specific heat coefficient (proportional to the density of states at the Fermi surface) between the ordered and disordered conditions. It was felt, in view of the unusual nature of the transformation in CuPt, that a similar investigation in CuPt would be of interest.

EXPERIMENTAL

Copper of 99.999% purity (Asarco A-58) and platinum sponge of 99.999% (Johnson-Mathey 1010) in the appropriate amounts were induction melted in a high-purity graphite crucible under a protective atmosphere of helium. The resulting ingot was homogenized in the crucible by holding between 1250° and 1350°C for 5 h. Chemical analysis showed no significant composition difference between the top and bottom of the ingot; the mean concentration of copper was 24.51 wt%, the stoichiometric composition being 24.57 wt%. A spectroscopic analysis showed Fe to be present at less than 4 ppm, and Mn and Co both less than 1 ppm. A cylindrical specimen slightly less than

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