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Note on the Convergence of the KROLL Method*

By

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The behavior of the KROLL solution of the BLOCH integral equation was studied at extreme low temperatures.

Recently TOYA and one of us (K.U.)[1] have investigated on the convergence of the KROLL solution of the BLOCH integral equation in the region of finite temperatures ($T/\Theta = 0.1$ to 10). The solution

$$c(\eta) = c_0 + c_1\eta + c_2\eta^2 + \cdots\cdots\cdots\cdots \tag{1}$$

seems to tend to an even function of η with decreasing temperature. This behavior is examined here more precisely at extreme low temperatures.

Since all coefficients a_{ij} and b_{ij} in the set of the fundamental equations (3) in I are composed from $J_n(x = \Theta/T)$ as given in Appendix of I and the latter behaves at extreme low temperatures in the following manner:

$$\left.\begin{aligned} &J_n(x \gg 1) = J_n(\infty) - e^{-x}x^n\,, \\ &dJ_n/dT\,(T \to 0) = 0\,, \end{aligned}\right\} \tag{2}$$

they can be taken as constant, i. e. $a_{ij}(T=0) \equiv a'_{ij}$ and $b_{ij}(T=0) \equiv b'_{ij}$, so that explicit T alone plays rôle for the behaviors of c_i's. Thus, it is convenient to write the set of the fundamental equations in the following form:

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* Supplement to the article "On the Convergence of the KROLL Method" by UMEDA and TOYA[1] which is cited in this note as I.

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$$\left.\begin{aligned}
\tau^2 \boldsymbol{a}'_{11}\boldsymbol{c}_0 + \gamma\tau \boldsymbol{a}'_{12}\boldsymbol{c}_1 + \tau^2 \boldsymbol{a}'_{13}\boldsymbol{c}_2 + \cdots\cdots\cdots &= \boldsymbol{b}_1, \\
\gamma\tau \boldsymbol{a}'_{12}\boldsymbol{c}_0 + \boldsymbol{b}'_{22}\boldsymbol{c}_1 + \gamma\tau \boldsymbol{a}'_{23}\boldsymbol{c}_2 + \cdots\cdots\cdots &= \boldsymbol{b}_2, \\
\tau^2 \boldsymbol{a}'_{13}\boldsymbol{c}_0 + \gamma\tau \boldsymbol{a}'_{23}\boldsymbol{c}_1 + \boldsymbol{b}'_{33}\boldsymbol{c}_2 + \cdots\cdots\cdots &= \boldsymbol{b}_3, \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots &
\end{aligned}\right\} \tag{3}$$

$$\tau \equiv \frac{1}{X} = 2^{1/3}\frac{T}{\Theta}, \quad \gamma \equiv \frac{k\Theta}{\zeta}\frac{1}{2^{1/3}}, \quad \gamma\tau = \frac{kT}{\zeta}.$$

By virtue of the identical relations:

$$\boldsymbol{a}_{1,2i}(x) = (1/2)\,\boldsymbol{b}_{2,2i}(x) \tag{4}$$

and

$$\begin{vmatrix} a_{11} & 0 & a_{13} & \cdots \\ 0 & a_{22} & 0 & \cdots \\ a_{13} & 0 & a_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix} = \begin{vmatrix} a_{11} & a_{13} & \cdots \\ a_{13} & a_{33} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} a_{22} & a_{24} & \cdots \\ a_{24} & a_{44} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix}, \tag{5}$$

the coefficients determinant is reduced into the following form of the order of T^2:

$$\boldsymbol{D} = \tau^2 \boldsymbol{a}'_{11}\left(1 - \frac{\gamma^2}{4}\right) \begin{vmatrix} \boldsymbol{b}'_{22} & \boldsymbol{b}'_{24} & \cdots \\ \boldsymbol{b}'_{24} & \boldsymbol{b}'_{44} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} \boldsymbol{b}'_{33} & \boldsymbol{b}'_{35} & \cdots \\ \boldsymbol{b}'_{35} & \boldsymbol{b}'_{55} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix}. \tag{6}$$

The simplest approximation of this expression broken off at $\boldsymbol{b}_{33}$ was given already by WILSON[(2)].

The peculiarities of the first row and column, i. e.

$$\boldsymbol{b}_{1,2i+1} = 0 \tag{7}$$

and Eq. (4), make the behaviors of $\boldsymbol{c}_0$ and $\boldsymbol{c}_1$ only exceptional.

$\boldsymbol{c}_0$ diverges in order of T^{-2}:

$$\begin{aligned}
\boldsymbol{c}_0(T \to 0) &= \frac{1}{\tau^2}\frac{1}{J_5(\infty)}\frac{1}{1-(\gamma^2/4)}, \\
&= 5.0627 \cdot 10^{-3}(\Theta/T)^2 \qquad \text{for copper,}
\end{aligned} \tag{8}$$

which holds for all degree of approximation.* The behavior of $\boldsymbol{c}_0$ was discussed originally by KROLL[(3)].

$\boldsymbol{c}_1$ diverges, however, in order of T^{-1}:

$$\begin{aligned}
\boldsymbol{c}_1(T \to 0) &= -\frac{1}{\tau}\frac{1}{J_5(\infty)}\frac{\gamma/2}{1-(\gamma^2/4)}, \\
&= -9.7587 \cdot 10^{-7}(\Theta/T) \qquad \text{for copper,}
\end{aligned} \tag{9}$$

* The degree of approximation means the number of terms in the polynomial approximating Eq. (1), e.g. the n-terms approximation corresponds to the n-terms polynomial.

which holds also for all degree of approximation.

Making $T \to 0$ in the equations with b_2, b_4, $\cdots\cdots$ in Eqs. (3) and taking the identical relation

$$\gamma\, a'_{1,2\iota} c_0 + b'_{2,2\iota} c_1 = 0 \tag{10}$$

into consideration, we find all the other odd coefficients to vanish:

$$c_3(T \to 0) = c_5(T \to 0) = \cdots\cdots = 0\,. \tag{11}$$

All the other even coefficients c_2, c_4, $\cdots\cdots$ at $T=0$ are determined by the set of equations with b_3, b_5, $\cdots\cdots$ in (1) at $T \to 0$:

$$\left.\begin{aligned} b'_{33}c_2 + b'_{35}c_4 + \cdots\cdots &= b_3 - J_5(\infty)^{-1}(1-\gamma^2/4)^{-1}(a'_{13} - (\gamma^2/2)a'_{23})\,, \\ b'_{35}c_2 + b'_{55}c_4 + \cdots\cdots &= b_5 - J_5(\infty)^{-1}(1-\gamma^2/4)^{-1}(a'_{15} - (\gamma^2/2)a'_{25})\,, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\,, \end{aligned}\right\} \tag{12}$$

which afford for them definite nonvanishing limiting values dependent upon the degree of approximation as given in the following table.

Deg. of app.	$c_2(T=0)$	$c_4(T=0)$	$c_6(T=0)$	$c_8(T=0)$	$c_{10}(T=0)$
3 or 4	$-4.0865 \cdot 10^{-3}$				
5 or 6	-5.0951	$1.3855 \cdot 10^{-5}$			
7 or 8	-5.8748	3.3357	$-0.81943 \cdot 10^{-7}$		
9 or 10	-6.5045	5.5180	-2.5297	$0.31560 \cdot 10^{-9}$	
11 or 12	-7.0284	7.7781	-5.0284	1.1873	$-8.5145 \cdot 10^{-13}$

γ^2 being very small, for example $9.362 \cdot 10^{-6}$ for copper, these values can be considered to hold for all monovalent metals. From this table we see that the value of the each coefficient converges monotonously, but not quickly enough to the definite limiting value with the increasing degree of approximation.

The parts of the curves of c_2, c_4, $\cdots\cdots$ *versus* T/Θ at extreme low temperatures, which were left, however, not drawn in Fig. 7 of I, are shown in Fig. 1, where they run sufficiently parallel to the T-axis owing to the property of J_n, Eq. (2) and their values except at $T=0$ were derived by solving directly the set of the fundamental equations (3) in I.

As the summary, it can be said that $c(\gamma)$ becomes a nearly even function in higher accuracy rather at $T/\Theta = 0.1$ to 0.3, than at extreme low temperatures, where c_1 diverges.

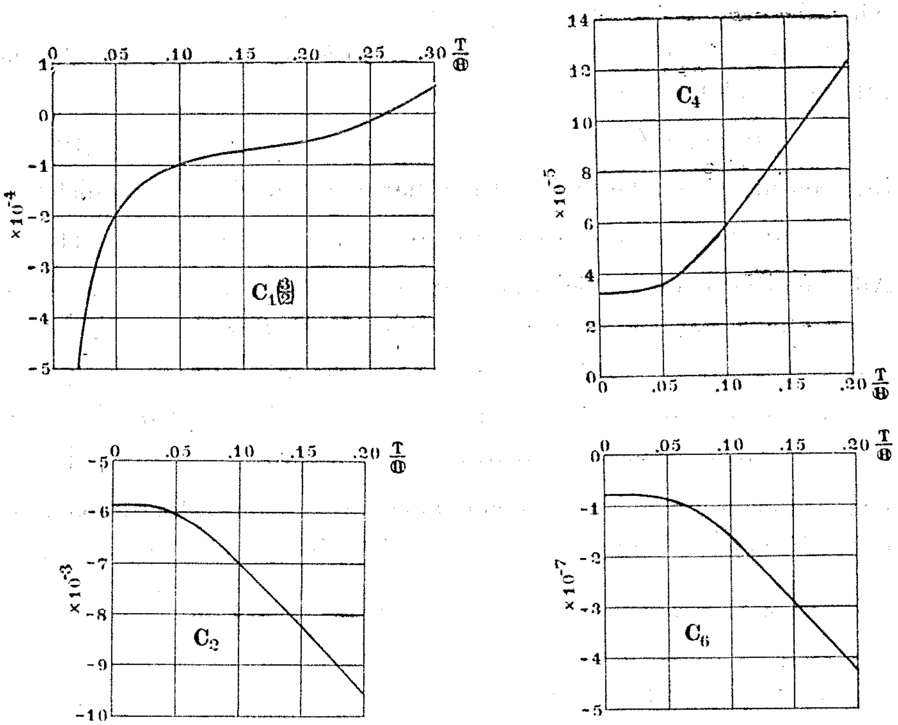

Fig. 1. c_1, c_2, c_4 and c_6 in the 7 or 8 terms approximation as functions of T/Θ.

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Appendix

The 11 or 12 terms approximation needs the following coefficients which are not yet given in Appendix of I.

$$I_{17} = (1-e^{-z})^{-1}\,[-272a_{15}z^2 - 4760a_{13}z^4 - 24752a_{11}z^6 - 48620a_9z^8 - 38896a_7z^{10} - 12376a_5z^{12} - 1360a_3z^{14} - 34a_1z^{16} - (1/18)\,z^{18}],$$

$$I_{18} = (1-e^{-z})^{-1}\,[36a_{17}z + 1632a_{15}z^3 + 17136a_{13}z^5 + 63648a_{11}z^7 + 97240a_9z^9 + 63648a_7z^{11} + 17136a_5z^{13} + 1632a_3z^{15} + 36a_1z^{17} + (1/19)\,z^{19}],$$

$$I_{19} = (1-e^{-z})^{-1}\,[-342a_{17}z^2 - 7752a_{15}z^4 - 54264a_{13}z^6 - 151164a_{11}z^8 - 184756a_9z^{10} - 100776a_7z^{12} - 23256a_5z^{14} - 1938a_3z^{16} - 38a_1z^{18} - (1/20)\,z^{20}].$$

$$a_{1,11} = 20a_9J_5 + 240a_7J_7 + 504a_5J_9 + 240a_3J_{11} + 20a_1J_{13} + (1/11)\,J_{15}.$$

$$b_{3,11} = 400a_9J_5 + 2160a_7J_7 + 2688a_5J_9 + 840a_3J_{11} + 48a_1J_{13} + (5/33)\,J_{15},$$

$$b_{5,11} = 960a_{11}J_5 + 7000a_9J_7 + 13248a_7J_9 + 7968a_5J_{11} + 1456a_3J_{13} + 56a_1J_{15} + (400/3003)\,J_{17},$$

$$b_{7,11} = 1680a_{13}J_5 + 1644a_{11}J_7 + 45280a_9J_9 + 45720a_7J_{11} + 17472a_5J_{13} + 2240a_3J_{15} + 64a_1J_{17} + (471/4004)J_{19},$$

$$b_{9,11} = 2560a_{15}J_5 + 33040a_{13}J_7 + 126784a_{11}J_9 + 194440a_9J_{11} + 127296a_7J_{13} + 34272a_5J_{15} + 3264a_3J_{17} + 72a_1J_{19} + (2303/21879)J_{21},$$

$$b_{11,11} = 3600a_{17}J_5 + 60000a_{15}J_7 + 309120a_{13}J_9 + 671760a_{11}J_{11} + 671840a_9J_{13} + 310080a_7J_{15} + 62016a_5J_{17} + 4560a_3J_{19} + 80a_1J_{21} + (61585/646646)J_{23}.$$

References.

(1) K. UMEDA and T. TOYA: *Journal of the Faculty of Science, Hokkaidô University*, II, **3** (1949), 257.

(2) A. H. WILSON: *The Theory of Metals* (Cambridge, 1936), p. 218; *Proc. Camb. Phil. Soc.*, **33** (1937), 371.

(3) W. KROLL: *ZS. f. Phys.*, **80** (1933), 50.

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[**Note added in proof**] Recently, a paper on the KROLL method by E. H. SONDHEIMER, *Proc. Roy. Soc. London*, A, **203** (1950), 75, came to the author's notice, in which the determinant transformation, Eq. (5), was likely used. We are indebted to Dr. SONDHEIMER for the reprint sent to us.