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On the Convergence of the Kroll Method

By

Kwai UMEDA and Tomiyuki TOYA

(Received March 15, 1949)

Solving directly Kroll's set of equations, the nature of the solution of Bloch's integral equation has been investigated. It is a slowly varying and nearly even function, as it was assumed. By means of the results, the degree of accuracy of the solution in polynomial has been tested by the degree of convergence of the variational expression of Bloch's integral equation towards the extremum. The polynomial of 7 or 8 terms seems to be a practically sufficient approximation.

To solve Bloch's integral equation, Kroll\textsuperscript{(1)} has transformed it into an infinite set of equations which enables the solution to be found in a power series systematically to any desired accuracy. In practice, however, it is impossible to solve an infinite set of equations, so that we have to take necessarily only a finite number of equations, that means to replace the power series by a polynomial. Then its degree of accuracy is to be questioned. Recently one of us (K.U.)\textsuperscript{(2)} has transformed Bloch's integral equation into a variational form which is expressed by means of the polynomial in $s$ terms for $c^{(m)}(\bar{s})$

$$c^{(m)}(\bar{s}) = c_0^{(m)} + c_1^{(m)}\bar{s} + c_2^{(m)}\bar{s}^2 + \cdots + c_{s-1}^{(m)}\bar{s}^{s-1} \quad (1)$$

in a very simple form as a function of $s$

$$b_1^{(m)}c_0^{(m)} + b_2^{(m)}c_1^{(m)} + \cdots + b_s^{(m)}c_{s-1}^{(m)} = \text{extremum}, \quad (2)$$

provided that $c_0^{(m)}, c_1^{(m)}, \ldots$ are the roots of Kroll's set of equations. This enables the questioned degree of accuracy of the polynomial to be determined by seeing how closer this variational expression \textsuperscript{(2)} does converge towards the maximum as the number of terms in the polynomial $s$ increases. This procedure provides at the same time

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\textsuperscript{*} Presented partly at the semiannual meeting of The Institute of Physical and Chemical Research in Tokyo, June 10 and December 11, 1942. The publication was delayed owing to the wartime external conditions.

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a method to test the convergence of the power series (1) or the validity of the Kroll method.

In order to evaluate the variational expression (2), it is primarily necessary to determine the values of \( c_o, c_1, \ldots \) by solving numerically for every temperature Kroll's set of equations, which is put in the case of monovalent metals for the convenience of computation into the following form, where only the ratio \( \theta/\zeta \) appears as the material constant of the individual metal.

\[
\sum_{j=1}^{s} F_{iji} (x) c_{j}^{(n)} = b_{j}^{(n)} \quad i = 1, 2, \ldots, s, \quad n = \frac{3}{2}, \quad \frac{5}{2},
\]

where

\[
F_{iji} (x) = b_{ij} (x) + \frac{1}{X^2} a_{ij} (x), \quad \frac{kT}{\zeta} a_{ij} (x),
\]

\[
i + j = \text{even} \quad i + j = \text{odd}
\]

\[
X = \frac{1}{2} x = \frac{1}{2} \theta \frac{T}{\zeta}, \quad x = \frac{\theta T}{\zeta}.
\]

\[
\begin{array}{ccccccccccc}
i & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
b_{i}^{(1)} & \frac{1}{2} \pi^2 \frac{kT}{\zeta}, & \frac{7}{10} \pi^4 \frac{kT}{\zeta}, & \frac{31}{14} \pi^6 \frac{kT}{\zeta}, & \frac{127}{10} \pi^8 \frac{kT}{\zeta}, \\
1, & \frac{1}{3} \pi^2, & \frac{7}{15} \pi^4, & \frac{31}{21} \pi^6, & \frac{127}{15} \pi^8, \\
\hline
b_{i}^{(2)} & \frac{5}{6} \pi^2 \frac{kT}{\zeta}, & \frac{7}{6} \pi^4 \frac{kT}{\zeta}, & \frac{155}{42} \pi^6 \frac{kT}{\zeta}, & \frac{127}{6} \pi^8 \frac{kT}{\zeta}, \\
& \frac{1}{3} \pi^2, & \frac{7}{15} \pi^4, & \frac{31}{21} \pi^6, & \frac{127}{15} \pi^8.
\end{array}
\]

These values follow from the neglection of \( (kT/\zeta)^2 \), which is at most of the order of \( 10^{-5} \) in the temperature range lower than \( 2\theta \), though there remain some more considerations for the second order phenomena.

\[
n_i (x) \equiv \int_{0}^{\infty} \frac{z^2 dx}{e^{z} - 1} \int_{-\infty}^{+\infty} \frac{\left( \eta + z \right)^{-i-1} \eta^{-i}}{(1 + e^z)(1 + e^{-z})} d\eta \quad i + j = \text{even},
\]

\[
\equiv \int_{0}^{\infty} \frac{z^2 dx}{e^{z} - 1} \int_{-\infty}^{+\infty} \frac{2\eta^{i+j} - \left( \eta + z \right)^{i} \eta^{-i} - \left( \eta + z \right)^{-i} \eta^{j}}{(1 + e^z)(1 + e^{-z})} d\eta \quad i + j = \text{odd},
\]

\[
b_{ij} (x) \equiv 2 \int_{0}^{\infty} \frac{z^2 dx}{e^{z} - 1} \int_{-\infty}^{+\infty} \frac{\eta^{i+j} - \left( \eta + z \right)^{i} \eta^{-i} - \left( \eta + z \right)^{-i} \eta^{j}}{(1 + e^z)(1 + e^{-z})} d\eta.
\]  

These integrals can be expressed by the radiation integrals \( J_n (x) \), as tabulated in the appendix. Our quantities in Gothic letters are related to the corresponding ones used by Kroll or in reference (2) in the following manner.
On the Convergence of the Kroll Method

\[ a_{ij} = \begin{cases} (k\theta)^{2D-1} a_{ij} & i+j \text{ even,} \\ a_{ij} & i+j \text{ odd,} \end{cases} \]

\[ b_{ij} = (2\pi)^{2} b_{ij}, \]

\[ b_{ij}^{(n)} = \zeta^{-n} b_{ij}^{(n)}, \]

\[ c_{ij}^{(n)} = \zeta^{-n+1} c_{ij}^{(n)}. \]

We have solved the set of equations (3) for every number of terms from \( s = 1 \) to \( s = 8 \) in the temperature range \( T/\theta = 0.1 - 2 \). The even coefficients \( c_0, c_2, c_4, c_6, \ldots \) converge monotonously to the final values, while the odd ones \( c_1, c_3, c_5, c_7, \ldots \) oscillatorily, as the number of terms \( s \) increases. Fig. 1 shows this situation for \( T/\theta = 0.5 \) as an example. The temperature dependence of these coefficients are traced in Fig. 2. At lower temperatures than the Debye temperature, the odd coefficients are markedly smaller compared to the even ones, as seen from the orders of magnitude given in Table I, so that the function \( c^{(m)}(\gamma) \) is nearly even, as Bloch\(^5\) has ever assumed. Due to the exceptionally large value of \( c_0 \) the function \( c^{(m)}(\gamma) \) is a slowly varying function, as it was also supposed. At the limit \( T \to 0 \), however, all the odd coefficients increase infinitely as \( T^{-1} \), whereas the even ones tend to the finite limiting values, except \( c_0 \) increases strongly infinitely as \( T^{-2} \).

Table I. Orders of magnitude of the coefficients of the power series (1) at several temperatures.

<table>
<thead>
<tr>
<th>( T/\theta )</th>
<th>( c_0 )</th>
<th>( c_1 )</th>
<th>( c_2 )</th>
<th>( c_3 )</th>
<th>( c_4 )</th>
<th>( c_5 )</th>
<th>( c_6 )</th>
<th>( c_7 )</th>
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<tr>
<td>2</td>
<td>10(10^{-1})</td>
<td>10(10^{-2})</td>
<td>(10^{-3})</td>
<td>10(10^{-5})</td>
<td>10(10^{-7})</td>
<td>10(10^{-9})</td>
<td>10(10^{-9})</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>10(10^{-2})</td>
<td>10(10^{-3})</td>
<td>(10^{-4})</td>
<td>10(10^{-6})</td>
<td>10(10^{-7})</td>
<td>10(10^{-8})</td>
<td>10(10^{-9})</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>10(10^{-3})</td>
<td>10(10^{-4})</td>
<td>(10^{-5})</td>
<td>10(10^{-7})</td>
<td>10(10^{-8})</td>
<td>10(10^{-9})</td>
<td>10(10^{-9})</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>10(10^{-4})</td>
<td>10(10^{-3})</td>
<td>(10^{-5})</td>
<td>10(10^{-5})</td>
<td>10(10^{-7})</td>
<td>10(10^{-9})</td>
<td>10(10^{-9})</td>
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Fig. 2. $c_0 \ldots c_7$ as functions of the temperature $T/\theta$. 
Now we can evaluate the variational expression (2) in every number of terms at every temperature. Fig. 3 shows the relative values of the variational expression (2) in 3 or 4 terms and in 5 or 6 terms at every temperature with respect to the value of (2) in 7 or 8 terms. That the curves of these three approximations diverge from each other at intermediate temperatures markedly larger than at lower and higher temperatures, indicates that the convergence of the Kroll method is relatively poor at intermediate temperatures. Since the discrepancy between the approximations in 5 or 6 terms and the one in 7 or 8 terms is at most 1%, the polynomial of 7 or 8 terms, i.e. the substitution of 7 or 8 equations for the infinite set of equations, should be an approximation with the practically sufficient accuracy.

Because the variational expression (2) is for $n = 3/2$ and $5/2$ respectively equivalent to the principal quantities $K_1$ and $K_3$, and the difference between $K_1$, $K_3$ and $K_9$ is too small to be shown in the figure, the temperature dependence of the variational expression (2), given in Fig. 4 by means of the obtained values of $b_i$ and $c_i$, represents at the same time that of $K_1$, $K_2$ and $K_3$,

$$b_1^{(m)}c_i^{(m)} + b_2^{(m)}c_i^{(m)} + \ldots = K_{m+n-2}, \quad m, n = \frac{3}{2} \text{ or } \frac{5}{2},$$

which determine several quantities in the conduction theory, e.g.
directly the electrical conductivity, and by their difference of the order \((kT/\zeta)\) the thermal conductivity, the thermoelectric power, the Thomson coefficient etc. as functions of the temperature. These practical applications of the obtained results will be given in the continued article.

In conclusion, we wish express our sincere thanks to Dr. Kroll who has stimulated us while his stay in Sapporo as the visiting lecturer. The financial supports of The Department of Education and The Hattori-Hôkôkai are gratefully acknowledged.

Appendix

\[ a_n \equiv \int_0^\infty \frac{\eta^n}{1 + e^\eta} d\eta = \left(1 - \frac{1}{2^n}\right) m! \zeta(m+1), \]

\[ \zeta(m) \equiv 1 + \frac{1}{2^m} + \frac{1}{3^m} + \frac{1}{4^m} + \ldots, \]

\[ a_1 = (1/12)\pi^2, \quad a_2 = (7/120)\pi^4, \quad a_3 = (31/252)\pi^6, \quad a_4 = (12/240)\pi^8, \quad a_5 = (611/1320)\pi^{10}, \]

\[ a_{11} = (1414477,32760)\pi^{12}, \quad a_{13} = (8192/12)\pi^{14}, \quad a_{15} = (118518239/8160)\pi^{16}. \]

\[ I_n \equiv \int_0^\infty \frac{\eta^n}{(1 + e^\eta)(1 + e^{-\eta} - x)} d\eta = \frac{1}{1 - e^{-x}} \left[ \int_0^\infty \frac{(\eta + x)^n - (\eta - x)^n}{1 + e^\eta} d\eta + \frac{\eta^{x+1}}{n+1} \right], \quad n = \text{even}, \]

\[ I_0 = (1 - e^{-x})^{-1} [1], \quad I_1 = (1 - e^{-x})^{-1} [- (1/2)x^2], \quad I_2 = (1 - e^{-x})^{-1} [4x^2 + (1/3)x^3], \quad I_3 = (1 - e^{-x})^{-1} [6x^2 - (1/4)x^3], \quad I_4 = (1 - e^{-x})^{-1} [8x^2 + 8x^3 + (1/5)x^5], \quad I_5 = (1 - e^{-x})^{-1} [-20x^2 - 10x^4 + (1/6)x^5], \quad I_6 = (1 - e^{-x})^{-1} [12x^2 + 40x^3 + 12x^4 + (1/7)x^7]. \]

\[ I_7 = (1 - e^{-x})^{-1} [- 42x^2 - 70x^4 - 14x^6], \quad I_8 = (1 - e^{-x})^{-1} [- 16x^2 + 112x^3 + 112x^5 + 16x^7 + (1/9)x^9], \]

\[ I_9 = (1 - e^{-x})^{-1} [- 72x^2 - 258x^4 - 168x^6 - 18x^8 + (1/10)x^{10}], \quad I_{10} = (1 - e^{-x})^{-1} [90x^2 + 240x^3 + 50x^5 + 240x^7 + 20x^9 + (1/11)x^{11}], \]

\[ I_{11} = (1 - e^{-x})^{-1} [- 120x^2 + 440x^3 + 572x^5 - 72x^7 + 440x^9 + 20x^{11} - (1/12)x^{12}], \quad I_{12} = (1 - e^{-x})^{-1} [24x^2 + 144x^3 + 1584x^5 + 1684x^7 + 24x^9 + (1/13)x^{13}], \]

\[ I_{13} = (1 - e^{-x})^{-1} [- 156x^3 + 1430x^5 - 572x^7 - 720x^9 + 24x^{11} + (1/14)x^{14}], \]

\[ I_{14} = (1 - e^{-x})^{-1} [284x^4 + 728x^6 + 2730x^8 + 4004x^{10} + 6864x^{12} + (1/15)x^{15}], \quad I_{15} = (1 - e^{-x})^{-1} [284x^4 + 4004x^6 + 728x^8 + 2730x^{10} + 4004x^{12} + (1/16)x^{16}], \]

\[ I_{16} = (1 - e^{-x})^{-1} [32x^4 + 1120x^6 + 8730x^8 + 8730x^{10} + 1120x^{12} + (1/17)x^{17}], \quad I_{17} = (1 - e^{-x})^{-1} [32x^4 + 1120x^6 + 8730x^8 + 8730x^{10} + 1120x^{12} + (1/17)x^{17}], \]

\[ I_{18} = (1 - e^{-x})^{-1} [32x^4 + 1200x^6 + 8730x^8 + 8730x^{10} + 1120x^{12} + (1/17)x^{17}]. \]
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\[ J_n(x) = \int_0^\infty \frac{x^3}{(e^x - 1)(1 - e^{-x})} \, dx, \quad x = \frac{\theta}{T}, \]

\[ J_\infty(x) = n! \zeta(n), \]

\[ J_0(\infty) = 1.24433+10^2, \quad J_1(\infty) = 5 08208\times10^2, \quad J_0(\infty) = 3.63 085\times10^2, \]

\[ J_9(\infty) = 2.920653\times10^4 \]

\[ J_7(\infty) = 3.55601\times10^4 \]

\[ J_9(\infty) = 5.10093\times10^4 \]

\[ J_{11}(\infty) = 1.216453\times10^4 \]

\[ J_{11}(\infty) = 5.10093\times10^4 \]

\[ a_{11} = J_0, \]

\[ a_{11} = (1/2) J_0, \]

\[ a_{11} = 4a_1 J_0 + (1/3) J_7, \]

\[ a_{14} = 6a_1 J_0 + (1/4) J_7, \]

\[ a_{15} = 8a_0 J_0 + 8a_1 J_7 + (1/6) J_{10}, \]

\[ a_{19} = 20a_0 J_0 + 16a_1 J_7 + (1/8) J_{12}, \]

\[ a_{21} = 12a_0 J_0 + 40a_1 J_7 + 12a_2 J_7 + (1/7) J_{14}, \]

\[ a_{28} = 42a_0 J_0 + 70a_1 J_7 + 14a_2 J_7 + (1/8) J_{16}, \]

\[ a_{30} = 16a_0 J_0 + 112a_1 J_7 + 112a_2 J_7 + 16a_3 J_7 \]

\[ a_{31} = (1/2) J_0, \]

\[ a_{32} = 4a_1 J_0 - (1/6) J_7, \]

\[ a_{33} = 14a_0 J_0 + (5/12) J_7, \]

\[ a_{34} = 8a_0 J_0 + 2a_1 J_7 - (1/20) J_9, \]

\[ a_{35} = 52a_0 J_0 + 22a_1 J_7 + (3/10) J_9, \]

\[ a_{36} = 12a_0 J_0 + 20a_1 J_7 + 2a_2 J_7 - (1/42) J_9, \]

\[ a_{37} = 11a_0 J_0 + 170a_1 J_7 - 30a_2 J_7 \]

\[ + (13/56) J_{12}, \]

\[ a_{38} = 16a_0 J_0 + 70a_1 J_7 - 42a_2 J_7 - 2a_3 J_7 \]

\[ + (1/72) J_{12}, \]

\[ a_{39} = 200a_0 J_0 + 64a_1 J_7 + 32a_2 J_7 + 32a_3 J_7 \]

\[ + (17/90) J_{12}, \]

\[ a_{40} = 8a_0 J_0 + (1/30) J_9, \]

\[ a_{41} = 68a_0 J_0 + 24a_1 J_7 + (17/60) J_9, \]

\[ a_{42} = 12a_0 J_0 + 8a_1 J_7 + (1/105) J_{11}, \]

\[ a_{43} = 162a_0 J_0 + 210a_1 J_7 - 32a_2 J_7 \]

\[ + (37/168) J_{11}, \]

\[ a_{44} = 16a_0 J_0 + 40a_1 J_7 + 12a_2 J_7 + (1/252) J_{12}, \]

\[ a_{45} = 292a_0 J_0 + 566a_1 J_7 - 402a_2 J_7 + 40a_3 J_7 \]

\[ + (13/72) J_{12}, \]

\[ a_{46} = 20a_0 J_0 + 112a_1 J_7 + 112a_2 J_7 + 16a_3 J_7 \]

\[ + (1/400) J_{12}, \]

\[ a_{47} = 12a_0 J_0 + 4a_1 J_7 - (1/140) J_{12}, \]

\[ \alpha_{46} = 186a_0 J_0 + 222a_1 J_7 + 32a_2 J_7 \]

\[ + (137/840) J_{12}, \]

\[ a_{48} = 5a_0 J_0 + 992a_1 J_7 - 9a_2 J_7 - (1/504) J_{12}, \]

\[ a_{49} = 36a_0 J_0 + 654a_1 J_7 + 478a_2 J_7 + 40a_3 J_7 \]

\[ + (51/280) J_{12}, \]

\[ a_{50} = 20a_0 J_0 + 72a_1 J_7 + 42a_2 J_7 + 2a_3 J_7 \]

\[ + (1/1320) J_{12}, \]

\[ a_{51} = 590a_0 J_0 + 280a_1 J_7 + 930a_2 J_7 \]

\[ + 878a_3 J_7 + 148a_4 J_7 + (183/1188) J_{12}, \]

\[ a_{52} = 16a_0 J_0 + 16a_1 J_7 + (1/630) J_{12}, \]

\[ a_{53} = 322a_0 J_0 + 992a_1 J_7 + 480a_2 J_7 + 40a_3 J_7 \]

\[ + (687/3780) J_{12}, \]

\[ a_{54} = 20a_0 J_0 + 48a_1 J_7 + 12a_2 J_7 + (1/2310) J_{12}, \]

\[ a_{55} = 670a_0 J_0 + 3012a_1 J_7 + 3160a_2 J_7 \]

\[ + 880a_3 J_7 + 48a_4 J_7 + (208/1290) J_{12}, \]

\[ a_{56} = 24a_0 J_0 + 120a_1 J_7 + 112a_2 J_7 + 16a_3 J_7 \]

\[ + (1/6435) J_{12}, \]

\[ a_{57} = 20a_0 J_0 + 40a_1 J_7 + 4a_2 J_7 - (1/2772) J_{12}, \]

\[ a_{58} = 710a_0 J_0 + 3100a_1 J_7 + 3166a_2 J_7 \]

\[ + 880a_3 J_7 + 43a_4 J_7 + (333/5544) J_{12}, \]

\[ a_{59} = 24a_0 J_0 + 90a_1 J_7 + 44a_2 J_7 + 2a_3 J_7 \]

\[ + (1/10296) J_{12}, \]

\[ a_{60} = 116a_0 J_0 + 7680a_1 J_7 + 13240a_2 J_7 \]

\[ + 8006a_3 J_7 + 1456a_4 J_7 + 58a_5 J_7 \]

\[ + (12013/93090) J_{12}, \]

\[ a_{61} = 24a_0 J_0 + 83a_1 J_7 + 24a_2 J_7 \]

\[ + (1/13021) J_{12}, \]

\[ a_{62} = 116a_0 J_0 + 7800a_1 J_7 + 13708a_2 J_7 \]

\[ + 8006a_3 J_7 + 1456a_4 J_7 + 58a_5 J_7 \]

\[ + (4804/360300) J_{12}, \]

\[ a_{63} = 28a_0 J_0 + 152a_1 J_7 + 124a_2 J_7 + 16a_3 J_7 \]

\[ + (1/45045) J_{12}. \]
\[ \alpha_{99} = 23a_{99}J_5 + 224a_{99}J_7 + 224a_{99}J_9 + 32a_{99}J_{11} + (1/218790)J_{21}, \]
\[ b_{11} = 1152a_{11}J_5 + 7760a_{11}J_7 + 1368a_{11}J_9 + (9604/45045)J_{19}, \]

References