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An Exact Solution of a Molecular Field Equation in the Theory of Ferromagnetism

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1. Introduction

In a recent series of papers [1–4], Siewert and Burniston have made use of the theory of complex variables to solve a class of transcendental equations basic to several areas of mathematical physics. The method of solution is based on the construction, by the methods of Muskhelishvili [5], of canonical solutions to appropriately posed Riemann problems [5] and yields ultimately closed-form results for the desired solution.

Here we wish to use the method to solve explicitly the equation

$$\zeta=\tanh\tfrac{1}{2}(j\,z\,\zeta+h) \tag{1}$$

that is of interest in the molecular field theory of ferromagnetism. Since equation (1) has been well discussed in the literature, for example by Weiss [6] and Heisenberg [7], we note simply that the reduced magnetization denotes

$$\zeta=\frac{2M}{N g\beta}, \tag{2}$$

where M is the magnetization of a sample of spin $\frac{1}{2}$ magnetic atoms, with density N atoms/cm^3, β denotes the Bohr magneton and g is the Landé factor. Further, the parameters j and h are given by

$$j=\frac{J}{kT} \quad \text{and} \quad h=\frac{g\beta H}{kT}, \tag{3}$$

where k is Boltzmann's constant, T is the absolute temperature, H is the external field, and the exchange integral J characterizes the interaction between z nearest neighbors in the molecular field approximation. We consider the parameters j, z, and h to be given and thus note that equation (1) is transcendental in ζ.

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2. Analysis

To solve equation (1) we find it convenient to introduce the variables

$$a=\tfrac{1}{2}jz, \quad b=\tfrac{1}{2}h, \quad \text{and} \quad \xi=\frac{1}{\zeta} \tag{4}$$

and consider the equivalent problem of seeking the zeros of

$$\Lambda(\xi)=a+b\,\xi-\xi\,\text{arctanh}\,\frac{1}{\xi}. \tag{5}$$

Though the parameters a and b are positive for the posed problem, we wish to allow all non-zero real values of a and b, for the sake of other possible applications. We dismiss the possibility that $a=0$ since equation (1) would then not be transcendental; the special case $b=0$ is of interest in neutron-transport theory and has been discussed [1]. Further, we seek here only the real solutions of equation (1), although for $a>0$, we will in fact, for some values of a and b, obtain two of the complex solutions. The fact that equation (1) can have either one or three real solutions, depending on a and b, can be deduced straightforwardly from graphical considerations. We note that our analysis yields all of the real solutions.

We note that $\Lambda(\xi)$, as a function of a complex variable and as given by equation (5), is multivalued; however, the representation

$$\Lambda(\xi)=a+b\,\xi+\tfrac{1}{2}\xi\int_{-1}^{1}\frac{dv}{v-\xi} \tag{6}$$

is clearly analytic in the complex plane cut along the real axis from -1 to 1. It is also evident that any zero ξ_α of $\Lambda(\xi)$ will yield a solution of equation (1). We now seek *all* zeros of $\Lambda(\xi)$, as defined by equation (6).

If in equation (6) we let ξ approach the branch cut from above $(+)$ and below $(-)$, we find that the resulting boundary values can be expressed as

$$\Lambda^{\pm}(t)=a+b\,t-t\,\text{arctanh}\,t\pm i\tfrac{1}{2}\pi t, \qquad t\in(-1,1). \tag{7}$$

Note that the boundary values $\Lambda^{\pm}(t)$ cannot vanish on the cut. The argument principle [8] can now be used to compute the number of zeros of $\Lambda(\xi)$ in the cut plane. By computing the change in the argument of $\Lambda(\xi)$ about two enclosing contours (one of which is a large circle, centered at the origin, which we allow to tend to infinity, and another that just encloses the cut, which we allow to shrink onto the cut) we find there to be two cases:

(1) $a<0$: $\Lambda(\xi)$ has 1 zero, say ξ_0.
(2) $a>0$: $\Lambda(\xi)$ has 3 zeros, say ξ_0, ξ_1, and ξ_2.

We first consider $a<0$ and thus note that

$$F(\xi)=\frac{\Lambda(\xi)}{\xi-\xi_0}, \qquad a<0, \tag{8}$$

is analytic and nonvanishing in the finite cut plane. We therefore conclude, on letting ξ approach the branch cut from above and below, that $F(\xi)$ is a canonical solution of the Riemann problem [5]

$$\Phi^{+}(t)=G(t)\,\Phi^{-}(t), \qquad t\in(-1,1), \tag{9}$$

where

$$G(t)=\frac{\Lambda^{+}(t)}{\Lambda^{-}(t)}=\exp\left[i\,2\arg\Lambda^{+}(t)\right] \tag{10}$$

is the Riemann coefficient. The work of Muskhelishvili [5] and Simonenko [9] allows us to write a canonical solution to this Riemann problem as

$$\Phi(\xi)=\left(\frac{\xi+1}{\xi-1}\right)\exp\left[\frac{1}{\pi}\int_{-1}^{1}\Theta_1(t)\frac{dt}{t-\xi}\right], \qquad a<0, \tag{11}$$

where

$$\Theta_1(t)=\tan^{-1}\left[\frac{\pi t}{2(a+b\,t-t\,\mathrm{arctanh}\,t)}\right] \tag{12}$$

is taken to be continuous and such that $\Theta_1(-1)=\Theta_1(1)=\pi$. Since canonical solutions of the Riemann problem can only differ by a multiplicative constant, we deduce, from the form of $F(\xi)$ and $\Phi(\xi)$ as $|\xi|\to\infty$, that

$$F(\xi)=b\,\Phi(\xi), \qquad a<0, \tag{13}$$

and subsequently, on using equations (8) and (11), we find the desired solution:

$$\xi_0=\xi-\frac{\Lambda(\xi)}{b\,\Phi(\xi)}, \qquad a<0, \tag{14}$$

or

$$\frac{1}{\zeta_0}=\xi-\frac{\Lambda(\xi)}{b}\left(\frac{\xi-1}{\xi+1}\right)\exp\left[-\frac{1}{\pi}\int_{-1}^{1}\Theta_1(t)\frac{dt}{t-\xi}\right], \qquad a<0. \tag{15}$$

Equation (15) constitutes our general solution for case (1). We observe that equation (15) is, in fact, an identity in the ξ plane and thus ξ can be assigned any convenient (for example, in regard to computations) value; the choice $|\xi|\to\infty$ yields the concise result

$$\frac{1}{\zeta_0}=2+\frac{1-a}{b}-\frac{1}{\pi}\int_{-1}^{1}\Theta_1(t)\,dt, \qquad a<0. \tag{16}$$

Now considering $a>0$, we observe that

$$F(\xi)=\frac{\Lambda(\xi)}{(\xi-\xi_0)(\xi-\xi_1)(\xi-\xi_2)}, \quad a>0, \tag{17}$$

is a canonical solution of the Riemann problem defined by equations (9) and (10), which can be solved for $a>0$ to yield

$$\Phi(\xi)=\frac{1}{\xi^2-1}\exp\left[\frac{1}{\pi}\int_{-1}^{1}\Theta_2(t)\frac{dt}{t-\xi}\right], \quad a>0, \tag{18}$$

where

$$\Theta_2(t)=\tan^{-1}\left[\frac{\pi t}{2(a+bt-t\,\mathrm{arctanh}\,t)}\right], \tag{19}$$

with $\Theta_2(t)$ being continuous and such that $\Theta_2(-1)=-\pi$ and $\Theta_2(1)=\pi$. Note that we have defined the argument of $\Lambda^+(t)$ differently for the two cases $a<0$ and $a>0$. Again since $\Phi(\xi)$ and $F(\xi)$ can differ by no more than a multiplicative constant, we can write

$$(\xi-\xi_0)(\xi-\xi_1)(\xi-\xi_2)=\frac{\Lambda(\xi)}{b\,\Phi(\xi)}, \quad a>0. \tag{20}$$

If we now evaluate equation (20) at three distinct points, say $\xi=\alpha$, $\xi=\beta$ and $\xi=\gamma$, with α, β, and γ real but $\notin[-1,1]$, then we can eliminate between the resulting three equations to obtain

$$\frac{\Lambda(\xi)}{b\,\Phi(\xi)}=\xi^3+A_2(\alpha,\beta,\gamma)\,\xi^2+A_1(\alpha,\beta,\gamma)\,\xi+A_0(\alpha,\beta,\gamma), \tag{21}$$

where

$$A_0(\alpha,\beta,\gamma)=-\alpha\beta\gamma+\beta\gamma(\beta-\gamma)\,T\Omega(\alpha)+\gamma\alpha(\gamma-\alpha)\,T\Omega(\beta)+\alpha\beta(\alpha-\beta)\,T\Omega(\gamma), \tag{22a}$$

$$A_1(\alpha,\beta,\gamma)=\alpha\beta+\beta\gamma+\gamma\alpha-(\beta^2-\gamma^2)\,T\Omega(\alpha)-(\gamma^2-\alpha^2)\,T\Omega(\beta)-(\alpha^2-\beta^2)\,T\Omega(\gamma), \tag{22b}$$

$$A_2(\alpha,\beta,\gamma)=-\alpha-\beta-\gamma+(\beta-\gamma)\,T\Omega(\alpha)+(\gamma-\alpha)\,T\Omega(\beta)+(\alpha-\beta)\,T\Omega(\gamma), \tag{22c}$$

$$\Omega(\xi)=-\frac{\Lambda(\xi)}{b\,\Phi(\xi)}, \quad \text{and} \quad T=[(\alpha-\beta)(\beta-\gamma)(\gamma-\alpha)]^{-1}. \tag{23}$$

It is thus clear that the three desired solutions ζ_0, ζ_1, and ζ_2 are the three roots of the cubic equation

$$A_0(\alpha,\beta,\gamma)\,\zeta^3+A_1(\alpha,\beta,\gamma)\,\zeta^2+A_2(\alpha,\beta,\gamma)\,\zeta+1=0, \tag{24}$$

which can, of course, be solved analytically. The coefficients $A_i(\alpha,\beta,\gamma)$ are defined constants; however, we note that the accuracy of a computational scheme based on equations (22) depends on the particular choices of α, β, and γ. To find solutions similar to equation (16) we can let α, β, and γ all tend to infinity, or alternatively we can note the form of equation (21) as ξ tends to infinity, to obtain special expressions for the coefficients:

$$A_0 = \frac{2-3a}{3b} + \frac{a-1}{b}(I_1 + \tfrac{1}{2} I_0^2) + I_2 - I_0 + I_0 I_1 + \tfrac{1}{6} I_0^3, \tag{25a}$$

$$A_1 = \left(\frac{a-1}{b}\right) I_0 + I_1 + \tfrac{1}{2} I_0^2 - 1, \tag{25b}$$

and

$$A_2 = \frac{a-1}{b} + I_0, \tag{25c}$$

where

$$I_\alpha = \frac{1}{\pi} \int_{-1}^{1} \Theta_2(t)\, t^\alpha \, dt. \tag{26}$$

In conclusion we note that ζ_0 is always a real solution of equation (1); however, for $a>0$, ζ_1 and ζ_2 can be real or complex. Further, it is clear that we have found all of the zeros of $\Lambda(\xi)$, as defined by equation (6), and that these zeros yield the desired real solutions, as well as two of the complex solutions for some values of a and b, of equation (1). On the other hand, should all of the complex solutions and/or complex a and b be of interest, then the analysis reported here could, no doubt, readily be generalized, in the manner discussed by Burniston and Siewert [2], to yield the required results. Finally a Gaussian integration procedure has been used to evaluate numerically our explicit solutions, for numerous cases, and accuracy to within eight significant figures was achieved quite straightforwardly.

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Abstract

The theory of complex variables is used to develop an exact closed-form solution of a transcendental equation basic to the molecular field theory of ferromagnetism. The analysis yields analytical expressions, in terms of elementary quadratures, for the reduced magnetization ζ as it depends on the temperature and magnetic field.

Zusammenfassung

Im Rahmen der Theorie komplexer Variabler wird für eine, der Molekularfeldtheorie des Ferromagnetismus' zugrunde liegenden transzendenten Gleichung, eine exakte Lösung in geschlossener Form entwickelt. Die Rechnung liefert analytische Ausdrücke, in Form elementarer Quadraturen, welche die reduzierte Magnetisierung als Funktion der Temperatur und des Magnetfeldes beschreiben.

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