Prog. Theor. Phys. Vol. 37 (1967), No. 6

## First-Order Self-Energy Expressed in the Form of a Continued Fraction

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March 29, 1967

In preceding papers,[1)-3)] we have given a general approach to the problem of random lattices. One of the most important conclusions obtained therein is that the average over all the possible configurations of impurity sites must be carried out strictly in order that some physical requirement be fulfilled. It has been shown as an example[2)] that, when said averaging procedure is correctly followed, the first-order self-energy becomes

$$\Sigma(1) = NVI(GV, c) = NV\{P_1(c) + P_2(c)GV + P_3(c)(GV)^2 + \cdots\}, \tag{1}$$

where $c$ is the concentration of impurity atoms, $N$ the number of all lattice sites, $V$ the difference between potentials of an impurity and a host atom and $G$ the true Green's function. The coefficients $P_s(c)$ are defined by means of a generating function as

$$g(x;c) = \log[1-c+c\cdot\exp(x)] = \sum_{s=1}^{\infty} P_s(c)x^s/s! \tag{2}$$

The first-order self-energy $\Sigma(1)$ has a dual symmetry in the sense that the final result is unique irrespective of the unperturbed state chosen as a starting point.

The aim of the present short note is to prove that the function $I(x;c)$ is expressed by a continued fraction in the form

$$I(x;c) = c + xf_1(x;c), \tag{3a}$$

$$f_1(x;c) = \frac{c(1-c)}{1-(1-2c)x+x^2 f_2(x;c)}, \tag{3b}$$

$$f_n(x;c) = \frac{n(n-1)c(1-c)}{1-n(1-2c)x+x^2 f_{n+1}(x;c)} \quad (n \geq 2). \tag{3c}$$

The significance of writing $\Sigma(1)$ by the use of a continued fraction consists in the fact that, the convergence of Eq. (1) for arbitrary $x$ and $c$ being not self-evident at all and the evaluation of numerical results of $\Sigma(1)$ being too complicated to obtain except for some simple models, it is highly required to give a full discussion of the convergence of $\Sigma(1)$ and a proper asymptotic form to approximate $\Sigma(1)$; for this purpose the expression by a continued fraction is quite convenient.

The proof is as follows. According to Wall,[4)] there is a theorem that the problem of expanding a power series

$$\mathscr{P}\left(\frac{1}{z}\right) = \sum_{n=0}^{\infty}(-1)^n c_n/z^{n+1} \tag{4}$$

into the $J$-fraction

$$\cfrac{1}{b_1+z-\cfrac{a_1}{b_2+z-\cfrac{a_2}{b_3+z\cdots}}} \tag{5}$$

is equivalent to the problem of obtaining a power series identity of the form

$$Q(x+y) = Q(x)Q(y) + a_1Q_1(x)Q_1(y) + a_1a_2Q_2(x)Q_2(y) + \cdots, \tag{6}$$

where the $a_n$ are constants different from zero, and

$$Q(z) = \sum_{n=0}^{\infty} c_n z^n/n! \qquad (c_0=1), \tag{7}$$

$$Q_r(z) = \sum_{n=r}^{\infty} k_{r,n} z^n/n! \qquad (k_{r,r}=1). \tag{8}$$

The coefficients $a_n$ in the $J$-fraction are the $a_n$ of Eq. (6) and the $b_n$ of the $J$-fraction are given by

$$b_1 = k_{0,1},\ b_{n+1} = k_{n,n+1} - k_{n-1,n},\ n=1,2,3,\cdots. \tag{9}$$

In order to use the mentioned theorem, $xf_1(x;c)$ in Eq. (3a) is rearranged as

$$\begin{aligned} xf_1(x;c) &= P_2(c)x+P_3(c)x^2+P_4(c)x^3+\cdots \\ &= c(1-c)\{x-c_1x^2+c_2x^3-\cdots\} \\ &= c(1-c)\mathcal{P}(x), \end{aligned} \tag{10}$$

where it is easily seen from the properties of $P_s(c)$ that[2]

$$c_n=(-1)^n\frac{P_{n+2}(c)}{P_2(c)}=\frac{P_{n+2}(1-c)}{P_2(c)}. \tag{11}$$

On regarding $x$ in Eq. (10) as $1/z$, $Q(z)$ defined by Eq. (7) is written as

$$\begin{aligned} Q(z) &= \frac{1}{P_2(c)}\frac{d^2}{dz^2}\log[c+(1-c)\exp(z)] \\ &= \exp(z)\{c+(1-c)\exp(z)\}^{-2}. \end{aligned} \tag{12}$$

The next thing to do is to expand $Q(x+y)$ in the form of Eq. (6) which is performed by making use of an identity

$$\begin{aligned} c+(1-c)\exp(x+y) &= \{c+(1-c)\exp(x)\} \\ &\times\{c+(1-c)\exp(y)\}+c(1-c) \\ &\times\{\exp(x)-1\}\{\exp(y)-1\}. \end{aligned} \tag{13}$$

Thus, the expansion is

$$\begin{aligned} Q(x+y) &= \exp(x+y)\{c+(1-c)\exp(x+y)\}^{-2} \\ &= Q(x)Q(y)\,[1+c(1-c)R(x)R(y)]^{-2} \\ &= Q(x)Q(y)\sum_{r=0}^{\infty}(-1)^r(r+1) \\ &\times\{c(1-c)R(x)R(y)\}^r, \end{aligned} \tag{14}$$

where

$$R(x)=\{\exp(x)-1\}\{c+(1-c)\exp(x)\}^{-1}. \tag{15}$$

By comparing Eq. (14) with Eq. (6) and remembering that $k_{n,n}$ must be 1 for any $n$, the following relations are reached:

$$Q_r(x)=Q(x)\{R(x)\}^r/r!, \tag{16}$$

$$\prod_{n=1}^{r}a_n=(-1)^r(r+1)(r!)^2\{c(1-c)\}^r. \tag{17}$$

An explicit form of $a_n$ is derived from Eq. (17) as

$$a_n=-n(n+1)c(1-c). \tag{18}$$

On the other hand, Eqs. (6), (15) and (16) show that $k_{r,n}$ is given by

$$\begin{aligned} k_{r,n} &= \left[\frac{d^n}{dx^n}Q_r(x)\right]_{x=0} \\ &= \left[\frac{1}{r!}\frac{d^n}{dx^n}\left\{x^r-\frac{1-2c}{2}(r+2)x^{r+1}+\cdots\right\}\right]_{x=0}. \end{aligned} \tag{19}$$

In order to know $b_n$, only $k_{n,n+1}$ is necessary, which is obtained directly from Eq. (19) as

$$k_{n,n+1}=-(1-2c)\frac{(n+1)(n+2)}{2} \tag{20}$$

and thus

$$\begin{aligned} b_{n+1} &= k_{n,n+1}-k_{n-1,n}=-(1-2c)(n+1), \\ b_1 &= -(1-2c). \end{aligned} \tag{21}$$

Since $f_n(x;c)$ in Eq. (3c) is written by the coefficients of the $J$-fraction (5) as

$$f_n(x;c)=\frac{-a_{n-1}}{1+b_nx+x^2f_{n+1}(x;c)}, \tag{22}$$

Eq. (3) is proved.

When $f_2(x;c)$ is approximated by $f_1(x;c)$, Eq. (3b) becomes a closed form and $I(x;c)$ is readily calculated; this is regarded as a first approximation, which reduces to the same result as that obtained by Taylor.[5] Detailed discussion of higher-order approximations and of the convergence problem will appear in a forthcoming paper.


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