Letters to the Editor

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Association Problem in Statistical Mechanics—Critique of the Treatment of H. S. Green and R. Leipnik

MICHAEL E. FISHER
Wheatstone Physics Laboratory, King's College, London, W. C. 2, England
AND
H. N. V. TEMPERLEY
Atomic Weapons Research Establishment, Aldermaston, Berkshire, England

IN a recent paper Green and Leipnik[1] have indicated how the evaluation of the grand partition function of a classical system of interacting particles can be reduced by the cell-cluster method to a lattice combinatorial problem which they call the *association problem*. They discuss the general problem mathematically and claim to solve exactly a particular two-dimensional association problem which is "comparable in difficulty to the Ising problem." This note points out that the claimed solution of this problem [GL(51) and GL, p. 140] is manifestly incorrect. The reason for the error is shown to be a fallacious assumption made when applying the general mathematical theory. The solutions quoted by Green and Leipnik for various one-dimensional association problems *are* correct, but these problems can be solved more readily by an elementary, direct argument.

As formulated by Green and Leipnik, the association problem for a lattice L_n of n vertices requires the evaluation of the generating function

$$F_n(c_0,c_1,c_2,\cdots) = \sum_{m_0,m_1,\cdots} N_n(m_0,m_1,m_2,\cdots)c_0^{m_0}c_1^{m_1}c_2^{m_2}\cdots, \quad (1)$$

where $N_n(m_0,m_1,m_2,\cdots)$ is the number of ways of attaching m_0 copies of an oriented geometric object K_0 consisting of linked vertices (not necessarily adjoining), m_1 copies of an object K_1, m_2 copies of an object K_2, $\cdots$ to the lattice L_n, so that every lattice point of L_n is covered by one and *only* one vertex of an object K_i. The object K_0 is conventionally taken as the single unlinked vertex

$$K_0 = (\times),$$

so that we may rewrite (1) as

$$F_n(c_0,c_1,c_2,\cdots) = c_0^n\Lambda_n(d_1,d_2,\cdots), \quad (2)$$

where

$$d_i = c_i/c_0^{v_i}. \quad (3)$$

In these formulas, v_i is the number of vertices of the object K_i and

$$\Lambda_n = \sum_{m_1,m_2,\cdots} M_n(m_1,m_2,\cdots)d_1^{m_1}d_2^{m_2}\cdots, \quad (4)$$

where $M_n(m_1,m_2,\cdots)$ is defined in the same way as $N_n(m_0,m_1,m_2,\cdots)$ except that the restriction that *every* lattice point of L_n must be covered is relaxed.

Green and Leipnik consider [GL, p. 135] a particular two-dimensional association problem which corresponds to distributing bonds or "dimers" over a plane p by q quadratic lattice[2] ($pq=n$). The geometric objects in this case are the nearest neighbor horizontal and vertical bonds

$$K_1 = (\times\!\frown\!\times) \quad \text{and} \quad K_2 = \begin{pmatrix}\times\\ \times\end{pmatrix}.$$

[GL denote the latter as K_q; see also the following]. Green and Leipnik claim to express the solution of this problem in terms of powers of the matrix [GL(50)]

$$\mathbf{N}(c_0,c_1,c_2) = \begin{bmatrix} c_0 & 1 & 0 & 0 \\ c_1 & 0 & c_0 & 1 \\ c_2 & 0 & 0 & 0 \\ 0 & 0 & c_2 & 0 \end{bmatrix}. \quad (5)$$

For a large lattice in which edge effects are negligible, their solution [GL(51)] amounts to

$$\lim_{n\to\infty} \frac{1}{n}\log\Lambda_n = \log\lambda(d_1,d_2), \quad (6)$$

where λ is the largest root of the equation

$$\lambda^4 = \lambda^3 + d_1\lambda^2 + d_2\lambda + d_2^2, \quad (7)$$

which is (essentially) the characteristic equation of (5). [The existence of the limit (6) follows from general principles and merely reflects the extensive properties of the lattice.] It is immediately apparent that (5) and (7) are not symmetric under exchange of c_1 and c_2 (or of d_1 and d_2) whereas such symmetry is clearly essential in (6). (Although for a *finite rectangular* lattice symmetry would not be expected.) This at once casts doubt on the validity of (5) and (7) (and in fact led us to investigate the matter). That these results are indeed erroneous may be demonstrated explicitly by expanding $\log\lambda$ as a power series in d_1 and d_2. From the characteristic equation (7), we obtain (for the largest root)

$$\log\lambda(d_1,d_2) = d_1 + d_2 - \tfrac{3}{2}(d_1^2+d_2^2) - 4d_1d_2 + (10/3)(d_1^3+d_2^3) + 15d_1^2d_2 + 16d_1d_2^2 + O(d^4), \quad (8)$$

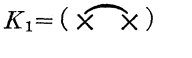
which shows that the expected lack of symmetry enters only in the third-order terms $d_1^2d_2$ and $d_1d_2^2$.

Now the exact expansion for $\log\lambda$ is easily calculated by direct enumeration of configurations on the lattice (regarded as wrapped on a torus). Thus,

$$\begin{aligned} &M_n(1,0)=M_n(0,1)=n,\\ &M_n(2,0)=M_n(0,2)=\tfrac{1}{2}n(n-3),\\ &M_n(1,1)=n(n-4),\\ &M_n(3,0)=M_n(0,3)=\tfrac{1}{6}n(n-4)(n-5),\\ &M_n(2,1)=M_n(1,2)=\tfrac{1}{2}n(n^2-11n+32). \end{aligned} \tag{9}$$

These relations confirm all terms of (8) except for $15d_1^2d_2$ which, in the exact expansion, is $16d_1^2d_2$. [The coefficients in (8) are, in the standard way, the coefficients of n in (9).]

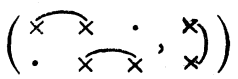
The matrix (5) is the same as that derived in GL(45)–(48) for the one-dimensional problem of nearest and next-nearest neighbors for which

$K_1=$ 

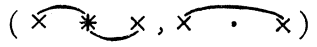
but

$K_2=$ 

[the dot indicates an unoccupied lattice point]. This matrix yields the correct solution of the one-dimensional problem (see the following) and will count configurations on the quadratic lattice correctly just as far as a one-one correspondence between the two sets of configurations can be set up. Examination shows that the first configuration on the quadratic lattice for which the correspondence breaks down is



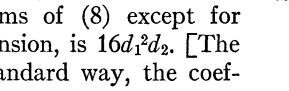
where the comma indicates that the vertical bond can be anywhere in the plane not overlapping the two horizontal bonds. On the one-dimensional lattice, this corresponds to the forbidden configuration



which has a doubly occupied vertex. The resultant difference accounts precisely for the change of the coefficients of $d_1^2d_2$ from 16 to 15.

Green and Leipnik's erroneous result can be traced to a false step in the application of a differential recurrence relation which they derived for an auxiliary generating function $R_r(x_1,x_2,\cdots;c_0,c_1,c_2,\cdots)$ which is simply related to the desired function (2). Their recurrence relation [GL(38)] is quite correct, although as we will indicate, it is not particularly useful. The difficulty is that for two-dimensional problems R_r is a polynomial in a *large number* of the variables x_j and is, *a priori*, of *unknown* degree.

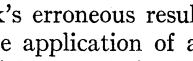
The problem on a general lattice may be restricted essentially to that on a one-dimensional lattice by using a suitable numbering system for the lattice points (see GL, p. 133). It then follows as observed in GL, that the number of variables x_j entering R_r is *at most* equal to the number of (horizontal) bonds separating the most distant vertices of the "longest" object under consideration. For a two-dimensional lattice of width q, an object which has any vertical extent will have a "length" which is near a *multiple* of q and hence (in the physically interesting limit $q\to\infty$) is indefinitely great. Thus, a nearest-neighbor vertical bond is equivalent to the "q bond"

$K_q=$ 

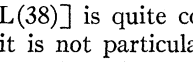
Consequently, for this case $R_r(x_1,x_2,\cdots;c_0,c_1,\cdots)$ might *a priori* depend on the q variables $x_1, x_2, \cdots, x_q$, although it is easily verified that R_1 depends *only* on x_1 and x_q. In their applications, Green and Leipnik (p. 136) have proceeded on the *assumption* that the same will be true for $R_2, R_3, \cdots, R_n$. Unless $q=2$, however, this is fallacious since it is readily verified by actual substitution in the recurrence relation [GL(38)] that R_2 depends explicitly on x_1, x_q, *and* x_{q-1}, R_3 on x_1, x_q, x_{q-1}, and x_{q-2}, $\cdots$, and R_q on $x_1, x_2, \cdots x_{q-1}, x_q$.

The fact that for a two-dimensional problem R_r will depend *explicitly* on an indefinitely large number of variables x_j seems to remove the essential basis for a successful approach along the lines Green and Leipnik propose. (Thus, their α [GL, p. 138] is of order $n!\to\infty$). Even for one-dimensional problems the GL method is difficult to apply due to the unknown degree of the polynomial $R_r(x_j)$ which leads to many "extraneous dimensions" [GL, pp. 135–136]. For example, for the problem with next-next-nearest neighbors ($q=3$), the fundamental characteristic equation is of degree eight (and is easily obtained by a method explained in the following) whereas with the GL approach, it seems essential to consider a 17×17 matrix.

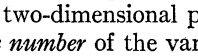
Green and Leipnik solved by their general methods a number of one-dimensional problems for which, more or less fortuitously, their generally fallacious assumption was in fact correct. These problems, however, yield readily to elementary methods. Consider the simplest example [GL, p. 134] of a linear lattice L_n of n points with nearest-neighbor bonds

$K_1=$  .

The configurations of L_n described by the generating function $F_n(c_0,c_1)$ must either terminate in a single vertex

$K_0=$ 

or in a bond

$K_1=$ 

and these correspond to factors c_0 and c_1, respectively. Consequently, we have the simple recurrence relation

$$F_n=c_0F_{n-1}+c_1F_{n-2} \tag{10}$$

whose solution is

$$F_n=A\lambda_1{}^n+B\lambda_2{}^n, \tag{11}$$

where λ_1 and λ_2 are roots of the characteristic equation

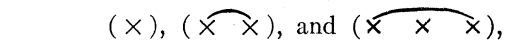
$$\lambda^2=c_0\lambda+c_1. \tag{12}$$

Imposition of the initial conditions $F_0=1$ and $F_1=c_0$ determines the arbitrary constants A and B and confirms GL(43).

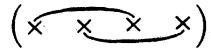
Consider now Green and Leipnik's second problem [GL, p. 135] which involves also next-nearest neighbors ($q=2$)

$K_2=$  .

Simple possible end configurations are



with corresponding factors c_0, c_1 and c_0c_2, but there is also the "overlapping" configuration

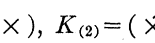


with factor $c_2{}^2$ which must not be overlooked. These four alternatives exhaust the possibilities so the recurrence relation can be written down directly. The characteristic equation is clearly

$$\lambda^4=c_0\lambda^3+c_1\lambda^2+c_0c_2\lambda+c_2{}^2, \tag{13}$$

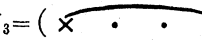
which is in agreement with GL(48) [compare also with (7) herein].

The linear lattice with the next-neighbor interactions [GL, p. 139]

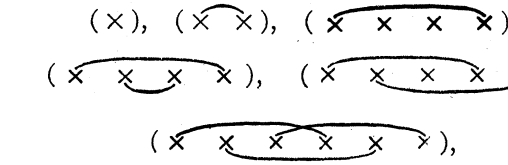
$K_{(1)}=$  , $K_{(2)}=$, $K_{(3)}=$, $\cdots$

is especially simple since there can be no overlapping configurations at the end of the chain. Green and Leipnik's characteristic equation [GL, p. 140] follows immediately.

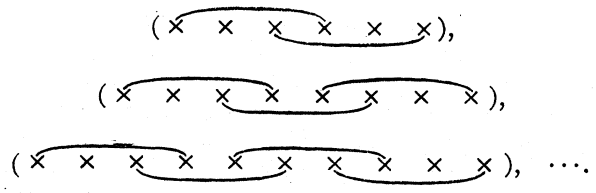
Finally, to illustrate the complications encountered in more difficult problems, consider the problem with next-next-nearest neighbors

$K_3=$ 

in place of next-nearest neighbors. This is the equivalent to a nearest-neighbor two-dimensional problem for a lattice of width $q=3$ with opposite edges joined to form a spiral. The list of possible end configurations is



and then an infinite series of overlapping configurations



This yields the recurrence relation

$$\begin{aligned}F_n=&c_0F_{n-1}+c_1F_{n-2}+(c_0{}^2+c_1)c_2F_{n-4}\\&+c_0c_3{}^2F_{n-5}+c_3{}^3F_{n-6}\\&+c_0{}^2c_3{}^2[F_{n-6}+c_3F_{n-8}+c_3{}^2F_{n-10}+\cdots],\end{aligned} \tag{14}$$

whence the characteristic equation is

$$\begin{aligned}\lambda^8=&c_0\lambda^7+(c_1+c_3)\lambda^6-c_0c_3\lambda^5+c_0{}^2c_3\lambda^4+c_0c_3{}^2\lambda^3\\&+c_3{}^2(c_3-c_1)\lambda^2-c_0c_3{}^2\lambda-c_3{}^4.\end{aligned} \tag{15}$$

This result can also be obtained from the GL approach if their assumption is corrected (i.e., if R_r is allowed to be a function of x_1, x_3, *and* x_2). The labor involved, however, is considerable and leads in the first place to a 17×17 matrix, since R_r appears to be cubic in x_1 and quadratic in x_2, and most cross terms such as $x_1{}^2x_2x_3$ must be allowed for.

The full two-dimensional case, however, does not yield to either of these approaches and still represents a challenging problem whose solution would be of interest for many applications of statistical mechanics.

[1] H. S. Green and R. Leipnik, Revs. Modern Phys. **32**, 129 (1960). Equations in this paper will be denoted GL(1), etc.

[2] Some aspects of this problem have been considered by A. J. Wakefield, D. Phil. thesis, Oxford, 1951.

On Green and Leipnik's Method for Solution of the Association Problem

SHIGETOSHI KATSURA AND SAKARI INAWASHIRO
Department of Applied Science, Tôhoku University, Sendai, Japan

RECENTLY Green and Leipnik[1] contributed a paper, "Exact Solution of the Association Problem by a Matrix-Spinor Method with Application to Statistical Mechanics," in which they described the method of obtaining the partition function of the association problem in one-, two-, and three-dimensional lattices. Unfortunately, their method is not effective and their solution is not correct in the problem of two and three dimensions. The exact solution still remained unsolved in explicit form.

According to their result, the two-dimensional association problem of the rectangular lattice with nearest-neighbor interaction is solved with a matrix

$$N(c_0,c_1,c_q)=\begin{bmatrix}c_0 & 1 & 0 & 0\\ c_1 & 0 & c_0 & 1\\ c_q & 0 & 0 & 0\\ 0 & 0 & c_q & 0\end{bmatrix},$$