AIP Journal of Mathematical Physics

Statistical Average of Product of Phase Sums Arising in the Study of Disordered Lattices. I

Priyamvada Sah

Citation: Journal of Mathematical Physics **10**, 2263 (1969); doi: 10.1063/1.1664832
View online: http://dx.doi.org/10.1063/1.1664832
View Table of Contents: http://scitation.aip.org/content/aip/journal/jmp/10/12?ver=pdfcov
Published by the AIP Publishing

be expected from Anderson's work.[13] It is possible to improve spin-wave theory still further, and investigations are in progress in which the coefficients in the canonical transformation are chosen to minimize the number of magnons in the true ground state. The main conclusion of this paper is that the large kinematic interaction found by recent authors at low temperatures can be understood as a nonphysical projection of the state vectors. This effect can be allowed for, and is relatively innocuous, as the eigenvalues of states with nonzero physical projection are physical. It is, therefore, still possible that the nonphysical eigenvalues may cancel out in the antiferromagnet, as they do in the ferromagnet at low temperature.

ACKNOWLEDGMENTS

The author wishes to thank Dr. S. Doniach for supervising this work. He is also indebted to the Science Research Council for the award of a research studentship.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 12 DECEMBER 1969

Statistical Average of Product of Phase Sums Arising in the Study of Disordered Lattices. I

PRIYAMVADA SAH
Department of Physics, Banaras Hindu University, Varanasi, India

(Received 27 January 1969)

A recurrence formula is established to evaluate the statistical average $\langle S(k_1)S(k_2)\cdots S(k_n)\rangle$ in the limit of $N\to\infty$, where $S(k)=\sum_{j=1}^{N} e^{ikx_j}$, $x_1, x_2, \cdots, x_N$, denotes the position of atoms in a disordered lattice, under the condition that interatomic distances are statistically independent and have the same probability distribution $s(r)$.

1. INTRODUCTION

If we consider the one-electron levels in a disordered array of atoms, the electronic energy levels depend on the position of atoms as parameters. The perturbation expansion of energy in certain approximations would involve the product of phase sums[1] and hence the formulas derived here are useful in evaluating the terms and may be of use in other connections also. Let $x_1, x_2, \cdots, x_N$ denote the positions of atoms from one end and $r_1, r_2, \cdots, r_N$ the interatomic distances. We define

$$S(k)=\sum_{j=1}^{N} e^{ikx_j} = e^{ikr_1}+e^{ik(r_1+r_2)}+\cdots+e^{ik(r_1+r_2+\cdots+r_N)}. \quad (1)$$

For any n,

$$S(k_1)S(k_2)\cdots S(k_n) = \sum_{K_1,K_2,\cdots,K_n} \exp\,[i(K_1r_1+\cdots+K_nr_n)], \quad (2)$$

where

$$K_1=k_1+k_2+\cdots+k_n, \quad (3)$$

and $K_2, \cdots, K_n$ are sums of any subset of $k_1, k_2, \cdots, k_n$ including the full set and empty set in such a way that the terms in $K_{\nu+1}$ are subset of terms in K_ν ($\nu = 1, 2, \cdots, N-1$). This restriction in forming the sum appearing in Eq. (2) will be called condition I. Denoting the left-hand side of (2) by $\Xi(N)$, we have

$$\Xi(N)=S(k_1)S(k_2)\cdots S(k_n). \quad (4)$$

The problem is to determine

$$\langle\Xi\rangle=\lim_{N\to\infty}\langle\Xi(N)\rangle.$$

We shall first derive $\langle\Xi(N)\rangle$, where N can be any number greater than n, and finally proceed to the limit as $N\to\infty$. This result is established under the assumption that none of $k_1, k_2, \cdots, k_n$ or their partial sums are zero. If any partial sum vanishes, the procedure has to be modified and will be considered later. These are needed in the complete discussion of perturbation terms.

In all terms of the right-hand side of Eq. (1) K_1 is fixed and given by Eq. (3), but $K_2, \cdots, K_n$ vary subject to condition I. Let us write

$$\Xi(N)=\Xi^{(1)}(N)+\Xi^{(2)}(N)+\cdots+\Xi^{n}(N), \quad (5)$$

so that, in every term of $\Xi^{(1)}(N)$, K_ν is either equal to K_1 or 0. In $\Xi^{(2)}(N)$, at least one of the $K_\nu = K_1^{(1)}$, where $0\subset K_1^{(1)}\subset K_1$. In $\Xi^{(j)}(N)$, K_ν assumes j distinct values $K_1, K_1^{(1)}, \cdots, K_1^{(j-1)}$. Every term in the rhs of Eq. (5)

[1] P. Sah, Ph.D. thesis, University of London, 1959.

is further subdivided:

$$\Xi^{(j)}(N) = \Xi_1^{(j)}(N) + \cdots + \Xi_{N-j+1}^{(j)}(N), \qquad j = 1, 2, \cdots, n, \quad (6)$$

where the subscript i in $\Xi_1^{(j)}(N)$ gives the number of K's which are equal to K_1. The highest possible subscript is $N - j + 1$ because, if the term has j distinct K's in it, the number of K's equal to K_1 cannot exceed $N - j + 1$.

2. DETERMINATION OF $\langle\Xi^{(j)}(N)\rangle$

$\langle\Xi^{(j)}(N)\rangle$ is now determined by induction. We assert that, for any $N \geq j$,

$$\langle\Xi^{(j)}(N)\rangle = P_j(K_1, K_1^{(1)}, \cdots, K_1^{(j-1)}) + Q_j(K_1, K_1^{(1)}, \cdots, K_1^{(j-1)}, N), \quad (7)$$

where P_j and Q_j are defined as follows:

$$P_j = \sum_{K_1, K_1^{(1)}, \cdots, K_1^{j-1}} \frac{f(K_1)}{1 - f(K_1)} \times \frac{f(K_1^{(1)})}{1 - f(K_1^{(1)})} \cdots \frac{f(K_1^{(j-1)})}{1 - f(K_1^{(j-1)})}, \quad (8)$$

where K_1 is given by Eq. (3) and $K_1^{(1)}, \cdots, K_1^{(j-1)}$ are all distinct. $K_1^{(i)}$, $i = 1, \cdots, (j-1)$, are partial sums of $k_1, k_2, \cdots, k_n$ in such a way that the terms of $K_1^{(i)} \subset K_1^{(i-1)}$, $i = 2, 3, \cdots, j-1$. This will be referred to as condition II. $f(K_1)$ is the Fourier transform of the probability distribution $s(r)$, i.e.,

$$f(K_1) = \int e^{iK_1 r} s(r)\, dr. \quad (9)$$

$s(r)$ is normalized and, therefore, $|f(K_1)| < 1$. The functions

$$Q_j(K_1, K_1^{(1)}, \cdots, K_1^{(j-1)}, N) = \sum_{K_1, \cdots, K_1^{(j-1)}} C_0^j f^N(K_1) + C_1^{(j)} f^N(K_1^{(1)}) + \cdots + C_{j-1}^{(j)} f^N(K_1^{(j-1)}), \quad (10)$$

where $C_i^{(j)}$, $i = (0, j-1)$, are some functions of $f(K_1), f(K_1^{(1)}), \cdots, f(K_1^{(j-1)})$, but do not depend on N. In writing $\langle\Xi^{(j)}(N)\rangle$ as $P_j + Q_j$, we have separated the parts which are dependent and independent of N.

To establish the basis for induction we show that the assertion is true for $j = 1$ and any $N \geq 1$. By definition,

$$\Xi^{(1)}(N) = e^{iK_1 r_1} + e^{iK_1(r_1+r_2)} + \cdots + e^{iK_1(r_1+r_2+\cdots+r_N)}. \quad (11)$$

The terms on the right are $\Xi_1^{(1)}, \Xi_2^{(1)}, \cdots, \Xi_N^{(1)}(N)$, respectively.

Since $r_1, r_2, \cdots, r_N$ are statistically independent, on averaging both sides of Eq. (11) we have, therefore,

$$\begin{aligned}\langle\Xi^{(1)}(N)\rangle &= f(K_1) + f^2(K_1) + \cdots + f^N(K_1) \\ &= \frac{f(K_1)}{1 - f(K_1)} - \frac{f(K_1)}{1 - f(K_1)} \cdot f^N(K_1) \\ &= P_1(K_1) + Q_1(K_1, N).\end{aligned}$$

P_1 and Q_1 have the postulated forms. We now show that the Eqs. (7), (8), and (10), which have been assumed for j, also hold for $j + 1$.

3. CORRESPONDENCE BETWEEN $\Xi^{(j)}(N - \mu)$ AND $\Xi_\mu^{(j+1)}(N)$

The nature of this correspondence can be brought out as follows. The terms of $\Xi^{(j)}(N)$ can be considered to arise from different arrangement of N objects $r_1, r_2, \cdots, r_N$ in j cells $K_1, K_1^{(1)}, \cdots, K_1^{(j-1)}$ which are the values of $K_1, K_2, \cdots, K_N$ appearing in Eq. (2). The cells are numbered from 1 to j and placed as shown in diagrams 1 and 2.

Objects	$r_1, r_2, \cdots, r_{\lambda_1}$	$r_{\lambda_1+1}, \cdots, r_{\lambda_2}$	$\cdots$	$r_{\lambda_{j-1}+1}, \cdots, r_{\lambda_j}$
Cell	K_1	$K_1^{(1)}$	$\cdots$	$K_1^{(j-1)}$

Diagram 1.

If $\lambda_j < N$, then $r_{\lambda_{j+1}} - r_N$ are undistributed.

The above diagram is replaced by a simpler diagram.

Object	$1, \cdots, \lambda_1$	$\lambda_1 + 1, \cdots, \lambda_2$	$\cdots$	$\lambda_{j-1} + 1, \cdots, \lambda_j$
Cell	1	2	$\cdots$	j

Diagram 2.

If $\lambda_j < N$, then $\lambda_j + 1, \cdots, N$ are undistributed. This diagram corresponds to a term

$$\exp\,[iK_1(r_1 + r_2 + \cdots + r_{\lambda_1}) + K_1^{(1)}(r_{\lambda_1+1} + \cdots + r_{\lambda_2}) + \cdots + K_1^{(j-1)}(r_{\lambda_{j-1}+1} + \cdots + r_{\lambda_j})]$$

in Eq. (2). There is at least one object in each cell, hence their number is $\leq N - (j-1)$ in any cell. Some may be left undistributed. All the terms of $\Xi^{(j)}(N)$ are obtained by assigning to $\lambda_1, \lambda_2, \cdots, \lambda_j$ all values compatible with the above conditions and $K_1^{(1)}, K_1^{(2)}, \cdots, K_1^{(j-1)}$ taking all values in accordance with condition II. In order to obtain arrangements which give rise to the terms of $\Xi^{(j+1)}(N)$, the cells are renumbered from 2 to $j+1$ and a new cell 1 is added in the front. The objects are rearranged in the new set of cells. This rearrangement is shown in diagram 3. r_1 always has the coefficient K_1 so it must be placed in cell 1, therefore it is taken from cell 2 and placed in cell 1. The number of objects in cells 2 to $j+1$ is restored by shifting them from cell p to $p-1$, $p=3,\cdots,j$ and in cell $j+1$ by drawing on undistributed objects as shown in diagram 3. Thus, to every arrangement in $\Xi^{(j)}(N)$ except those in which all objects are distributed, there corresponds one arrangement in $\Xi_1^{(j+1)}(N)$. It is clear that there is one-to-one correspondence between the terms in $\Xi^{(j)}(N-1)$ and $\Xi_1^{(j+1)}(N)$.

Objects	$1,\cdots,\lambda_1$	$\lambda_1+1,\cdots,\lambda_2$	$\lambda_2+1,\cdots,\lambda_3$	$\cdots$	$\lambda_{j-1}+1,\cdots,\lambda_j$	$:\Xi^j(N)$
Cells	1	2	3	$\cdots$	j	

$\lambda_j+1,\cdots,N$ undistributed

Objects	1	$2,\cdots,\lambda_1+1$	$\lambda_1+2,\cdots,\lambda_2+1$	$\lambda_2+2,\cdots,\lambda_3+1$	$\cdots$	$\lambda_{j-1}+2,\cdots,\lambda_j+1$	$:\Xi_1^{(j+1)}(N)$
Cells	1	2	3	4	$\cdots$	$j+1$	

$\lambda_j+2,\cdots,N$ undistributed.

Diagram 3.

Similarly, a one-to-one-correspondence exists between the terms of $\Xi^{(j)}(N-\mu)$ and $\Xi_\mu^{(j+1)}(N)$.

4. EVALUATION OF $\langle\Xi^{(j+1)}(N)\rangle$

Replacing j by $j+1$ in Eq. (6) gives

$$\langle\Xi^{(j+1)}(N)\rangle = \langle\Xi_1^{(j+1)}(N)\rangle + \cdots + \langle\Xi_{N-j}^{(j+1)}(N)\rangle,$$

and $\langle\Xi_1^{(j+1)}(N)\rangle$ can be obtained from $\langle\Xi^{(j)}(N-1)\rangle$ by replacing $K_1, K_1^{(1)},\cdots,K_1^{(j+1)}$ by $K_1^{(1)},\cdots,K^{(j)}$ (equivalent to relabeling) and multiplying the entire expression by $f(K_1)$, which is equivalent to putting object 1 in the newly added cell 1 in $\langle\Xi_1^{(j+1)}(N)\rangle$. Therefore, by (7), we have

$$\langle\Xi_1^{(j+1)}(N)\rangle = f(K_1)\{P_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)} + Q_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}, N-1)\}. \quad (12)$$

Similarly,

$$\langle\Xi_2^{(j+1)}(N)\rangle = f^2(K_1)\{P_j(K_1^{(1)},\cdots,K_1^{(j)}) + Q_j(K_1^{(1)},\cdots,K_1^{(j)}, N-2)\} \quad (13)$$

and, finally,

$$\langle\Xi_{N-j}^{(j+1)}(N)\rangle = f^{N-j}(K_1)\{P_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}) + Q_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}, j)\}. \quad (14)$$

It follows that the minimum value of N in $\langle\Xi^{(j+1)}(N)\rangle$ is $j+1$.

Using Eqs. (6), (12), (13), and (14), we have

$$\begin{aligned}\langle\Xi^{(j+1)}(N)\rangle &= P_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}) \\ &\quad\times\{f(K_1)+f^2(K_1)+\cdots+f^{N-j}(K_1)\} \\ &\quad+f(K_1)Q_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}, N-1) \\ &\quad+f^2(K_1)Q_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}, N-2) \\ &\quad+\cdots+f^{N-j}(K_1)Q_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}, j). \quad (15)\end{aligned}$$

One term $C_1^{(j)}f^N(K_1^{(1)})$ of Q_j in Eq. (10) will give the sum

$$\begin{aligned}C_1^{(j)}\{f(K_1)f^{N-1}(K_1^{(1)}) + f^2(K_1)f^{N-2}(K_1^{(1)}) &+\cdots+f^{N-j}(K_1)f^j(K_1^{(1)})\} \\ &= e_1 f^N(K_1^{(1)}) + e_2 f^N(K_1),\end{aligned}$$

where e_1 and e_2 do not depend on N. Hence the sum in Eq. (10) will give terms which can be put in the form

$$\sum_{K_1^{(1)},\cdots,K_1^{(j)}}\{C_0'^{(j+1)}f^N(K_1) + C_1^{(j+1)}f^N(K_1^{(1)}) + \cdots + C_j^{(j+1)}f^N(K_1^{(j)}, j)\}, \quad (16)$$

where $C_0'^{(j+1)}, C_1^{(j+1)},\cdots,C_j^{(j+1)}$ are independent of N. Their explicit form is not needed for the present purpose because in the limit of large N this sum will vanish:

$$\begin{aligned}\langle\Xi^{(j+1)}(N)\rangle &= P_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)}) \\ &\quad\times[f(K_1)-f^{N-j+1}(K_1)]/[1-f(K_1)] \\ &\quad+\sum_{K_1,\cdots,K_1^{(j)}}\{C_0^{(j+1)}f^N(K_1) \\ &\quad+C_1^{(j+1)}f^N(K_1^{(1)})+\cdots+C_j^{(j+1)}f^N(K_1^{(j)})\}.\end{aligned}$$

Therefore,

$$\begin{aligned}P_{j+1}(K_1, K_1^{(1)},\cdots,K_1^{(j)}) &= P_j(K_1^{(1)}, K_1^{(2)},\cdots,K_1^{(j)})f(K_1)/[1-f(K_1)] \\ &= \sum_{K_1,K_1^{(1)},\cdots,K^{(j)}}\frac{f(K_1)}{1-f(K_1)}\,\frac{f(K_1^{(1)})}{1-f(K_1^{(1)})}\cdots\frac{f(K_1^{(j)})}{1-f(K_1^{(j)})}\end{aligned} \quad (17)$$

and $Q_{j+1}(N)\to 0$ as $N\to\infty$.

5. CALCULATION OF $\langle \Xi(N) \rangle$

$$\langle \Xi(N)\rangle = \{P_1(K_1) + Q_1(K_1, N)\} + \{P_2(K_1, K_1^{(1)}) + Q_2(K_1, K_1^{(1)}, N)\} + \cdots + \{P_n(K_1, K_1^{(1)}, \cdots, K_1^{(n-1)}) + Q_n(K_1, K_1^{(1)}, \cdots, K_1^{(n-1)}, N)\}. \quad (18)$$

In the limit $N \to \infty$,

$$\lim_{N\to\infty} \langle \Xi(N)\rangle = \langle \Xi \rangle = \langle S(k_1)S(k_2)\cdots S(k_n)\rangle = \sum_{K_1} \frac{f(K_1)}{1-f(K_1)} + \sum_{K_1, K_1^{(1)}} \frac{f(K_1)}{1-f(K_1)} \frac{f(K_1^{(1)})}{1-f(K_1^{(1)})} + \cdots + \sum_{K_1,\cdots,K_1^{(n-1)}} \frac{f(K_1)}{1-f(K_1)} \cdots \frac{f(K_1^{(n-1)})}{1-f(K_1^{(n-1)})}. \quad (19)$$

This formula gives the average $\langle S(k_1)S(k_2)\cdots S(k_n)\rangle$ in the limit $N \to \infty$ in terms of the Fourier transform of the probability distribution of interatomic distances.

We will now express Eq. (19) as a recurrence formula. This is also more suitable for the actual computation of $\langle S(k_1)S(k_2)\cdots S(k_n)\rangle$ as a function of $k_1, k_2, \cdots, k_n$. Since K_1 is fixed,

$$\langle S(k_1)S(k_2)\cdots S(k_n)\rangle = \frac{f(K_1)}{1-f(K_1)}\Bigg(1 + \sum_{K_1^{(1)}} \frac{f(K_1^{(1)})}{1-f(K_1^{(1)})} + \sum_{K_1^{(1)},K_1^{(2)}} \frac{f(K_1^{(1)})}{1-f(K_1^{(1)})} \frac{f(K_1^{(2)})}{1-f(K_1^{(2)})} + \cdots + \sum_{K_1^{(1)},\cdots,K_1^{(n-1)}} \frac{f(K_1^{(1)})}{1-f(K_1^{(1)})} \times \frac{f(K_1^{(2)})}{1-f(K_1^{(2)})} \cdots \frac{f(K_1^{(n-1)})}{1-f(K_1^{(n-1)})}\Bigg). \quad (20)$$

From condition II, $K_1^{(1)}$ in the first sum can be the sum of $1, 2, \cdots, n-1$ elements among $k_1, k_2, \cdots, k_n$. Those $K_1^{(1)}$ which are equal to one element occur only in this term since only those $K_1^{(1)}$ which have nonnull subsets can appear in higher sums. From Eq. (20), their sum is $\sum_{i=1}^{n} \langle S(k_i)\rangle$. Those $K_1^{(1)}$ which are a sum of two terms appear in this sum and the second sum. These terms can be combined giving

$$\sum \frac{f(K_1^{(1)})}{1-f(K_1^{(1)})}\left(1 + \sum_{K_1^{(2)}} \frac{f(K_1^{(2)})}{1-f(K_1^{(2)})}\right),$$

where $\sum$ means that $K_1^{(1)}$ is the sum of any two k's from $k_1, k_2, \cdots, k_n$ and $\sum_{K_1^{(2)}}$ means that sum over $K_1^{(2)}$ subject to condition II, i.e., it is different from $K_1^{(1)}$ and 0, and it is a sum of subset of terms of $K_1^{(1)}$. These give rise to $\sum_{i,j=1}^{\prime n} \langle S(k_i)S(k_j)\rangle$. Those $K_1^{(1)}$ which are sum of $(n-1)$ k's occur in the second, third, $\cdots$, nth terms and the collection of all these is

$$\sum_{i,j,\cdots,l}' \langle S(k_i)S(k_j)\cdots S(k_l)\rangle.$$

We thus obtain the recurrence formula

$$\langle S(k_1)S(k_2)\cdots S(k_n)\rangle = \frac{f(k_1+\cdots+k_n)}{1-f(k_1+k_2+\cdots+k_n)}\Bigg[1 + \sum_{i=1}^{n} \langle S(k_i)\rangle + \sum_{i,j=1}^{\prime n} \langle S(k_i)S(k_j)\rangle + \cdots + \sum_{i,j,\cdots,l=1}^{\prime n} \langle S(k_i)S(k_j)\cdots S(k_l)\rangle\Bigg]. \quad (21)$$

There are n terms within the bracket which involve the mean value of S and its twofold, threefold, $\cdots$, $(n-1)$-fold products. The mean value of S can be found by putting $n = 1$. This result is then used to obtain the mean of twofold products which is given in terms of mean of S. To calculate the mean of the n-fold product of S, the mean of S, and its twofold, threefold, $\cdots$, $(n-1)$-fold products will have to be calculated successively by using Eq. (21). An extension of this result when k's are such that some partial sums vanish will be given in a later publication.