Russian Chemical Reviews

August 1983

Translated from *Uspekhi Khimii*, 52 1251-1262 (1983)

U.D.C. 530.145

# Correlation Functions of One-dimensional Systems

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The calculation of correlation functions describing the structure in space of one-dimensional systems is discussed, and various approaches to this problem are analysed. Examples of the use of correlation functions to interpret experimental X-ray and neutron scattering data and to calculate transition temperatures in quasi-one-dimensional systems are given.
The bibliography includes 41 references.

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## I. INTRODUCTION

In the light of recent advances in the synthesis of interesting quasi-one-dimensional compounds such as electrically conducting donor–acceptor complexes based on tetracyanoquinonedimethane (TCNQ),[1] polyacetylene doped with donors or acceptors[2], etc. the practical importance of one-dimensional physics is now self-evident. We know that one-dimensional system have a number of special attributes which produce a striking difference between one-dimensional and three-dimensional systems. In particular, and in spite of the relative simplicity of the one-dimensional systems, the well tried approximations used in the solution of three-dimensional problems are not always applicable to one-dimensional problems, and advances in one-dimensional physics must await the development of new methods.

Though theoretical studies of one-dimensional quantum systems began before the last war, detailed and organised work only began in the 1960's under the stimulus of successes in the preparation of these materials. During this period, which extends over 10–15 years, theoretical efforts were aimed mainly at the development of methods of calculating the energy characteristics (ground state energy, excitation spectra, etc.) and the thermodynamic parameters of one-dimensional systems. Approximate methods of calculating energies (by the specific variational method) were obtained, and allowed the energy of one-dimensional systems to be calculated very accurately[3]. Furthermore, for some one-dimensional models accurate results were obtained by a method which follows from the work of Bethe[3]. Numerical studies of systems consisting of a finite number of particles have also been very useful[4].

The main outcome of all this work was a realisation of the importance and of the specific features of correlation effects in one-dimensional systems, and the development of accurate methods of allowing for these effects. In spite of the continuing uncertainties in our understanding of some aspects of the energy characteristics (for example, the accurate correction for electron–phonon interactions, and in particular

† This and the following reviews are based on plenary papers presented to the Twelfth All-Union Congress on Organic Semiconductors (October 1982).

for the Peierls transition[5]), the energy problem can be considered (on the whole) to have been solved, and the main focus of attention is now a problem of a different kind: the calculation of the correlation functions of one-dimensional systems.

The correlation functions are different types of average over the wave functions of the system, which characterise its spatial structure as well as determining its response to various external stimuli (in particular, the diffraction of X-rays or neutrons by the system). The information contained in the correlation function is much more profuse than that implicit in a knowledge of the energy spectrum or of the thermodynamics of the system. As an example, we note that the most accurate calculations of the extent of charge transfer in quasi-one-dimensional donor–acceptor crystals of the TTF–TCNQ type (where TTF is tetrathiofulvalene) were based on diffuse X-ray and neutron diffraction spectra[6,7]. However, we should stress that the calculation of correlation functions is a much more complex problem than the calculation of energies. This is mainly because the former requires a knowledge of the wave functions of the system, and whereas the variational method gives acceptable results in calculations of energy it is far from satisfactory when applied to the calculation of wave functions. The method of Bethe, mentioned above, also gives accurate values of the energy but is unacceptable as a method of calculating wave functions. These difficulties are responsible for the lack (until recently) of serious attempts to calculate the correlation functions of one-dimensional systems, although accurate results were obtained[8,9] for a few, isolated model systems. The work done in the first stage has been expertly reviewed (see, for example, Ref.10), and is fully understood by theoreticians as well as by experimental scientists; on the other hand the problem of calculating correlation functions, which has been actively investigated only during the past 6–8 years, is still far from being solved, and has not yet been reviewed in detail. The various approaches to the solution of this problem are based on hypotheses which are difficult to prove and not always well founded, and therefore the acceptance of results from various laboratories is not universal. The aim of this paper is to review recent progress in this field and to discuss the results obtained so far.

## II. CORRELATION FUNCTIONS OF THE CONTINUUM MODEL OF A FERMI GAS

We shall examine most closely two specific correlators (or correlation functions): the one-particle density matrix $\rho(R)$, defined by the integral

$$\rho(R) = \rho \int \Psi^*(R, x_2, \ldots x_N)\, \Psi(0, x_2, \ldots, x_N)\, \mathrm{d}x_2 \ldots \mathrm{d}x_N$$

[where $\Psi(x_1, \ldots, x_N)$ is the wave function of the system, depending on the coordinates of the particles $(x_1, \ldots, x_N)$], and the pair correlation function $G(R, t)$,

$$G(R, t) = \langle \rho(0, 0)\, \rho(R, t) \rangle$$

where $\rho(R, t)$ is a density operator depending on the time $t$, and the angle brackets denote statistical averaging. The function $G(R, t)$ defines the probability of finding any particle of the system at a distance $R$ from the given particle at time $t$. In particular, for $t = 0$ and zero temperature ($T = 0$) we can write

$$G(R, 0) = \rho^2 \int \Psi^*(0, R, x_3, \ldots, x_N)\, \Psi(0, R, x_3, \ldots, x_N)\, \mathrm{d}x_3 \ldots \mathrm{d}x_N .$$

The correlator $\rho(R)$ is interesting because its Fourier transform $n(k)$ is a function of the distribution of the particles in momentum $k$ at $T = 0$. Also important is the Fourier transform of the correlator $G(R, t)$ (the dynamic form-factor $S(k, \omega)$, where $\omega$ is the frequency[11]), which determines the probability of scattering of neutrons and X-rays. We shall be mainly interested in the values of these correlators for large distances and long times.

The most characteristic feature of one-dimensional systems is the lack of long-range order even at $T = 0$, with a few exceptions, which will be mentioned below. This means that the value of the correlators is an inverse function of distance. The determination of this function is one of the theoretical problems facing us. In other words, we have the asymptotic laws $\rho(R) \propto R^{-\kappa}$ and $G(R, 0) \propto R^{-\alpha}$, and we are required to find $\kappa$ and $\alpha$ (which are sometimes called the critical indices).

It could be useful to dwell briefly on one aspect of the lack of long-range order in one-dimensional systems: the one-dimensional superconductor problem. It is often stated in the literature that one-dimensional superconductivity is impossible owing to the lack of long-range order. These statements rely on the analogy with a Bose gas, in which super-fluidity occurs as a result of a phase transition in the Bose condensate state whose matrix (or, more accurately, the non-diagonal elements of whose matrix) do not vanish for $R \to \infty$. We should stress that there is as yet no strict proof that one dimensional superconductivity is impossible in the absence of long-range order, and furthermore that metastable states with a non-zero current can exist in one-dimensional systems. Though phase transitions at $T \neq 0$ are impossible in one-dimensional systems, and these metastable states do not contribute long-range order, their life-times can be very long because states with a non-zero current and states with a zero current are separated by high activation barriers, and the probability of transitions between the two states is calculated[12] to be very small.

Two main approaches to the calculation of correlation functions are available at present. It has been assumed[13] that the behaviour of the correlation functions of one-dimensional Fermi systems (with which we shall be concerned in this review) at large distances is determined by gap-free long-wave excitations of the acoustic type (which are in fact responsible for the breakdown of long-range order). By allowing for these excitations and ignoring all the others we can obtain explicit expressions for the correlation functions.

The other approach to the calculation of correlators relies on the linearisation of the quadratic Fermion spectrum, i.e. on the replacement of $k^2/2m$ by $v_F k$ (where $m$ is the mass of the Fermion and $v_F$ is the Fermi velocity) and on the definition of two kinds of particle with $k = k_F$ and $k = -k_F$ respectively (where $k_F$ is the Fermi momentum, related to the particle density $\rho$ by the expression $k_F = \pi\rho$). Within the limitations of the "linear model" thus obtained, accurate calculations are possible[14–16].

The correlation functions obtained by these two approaches are qualitatively consistent. Their most characteristic features are the power-law decrease at large distances and the smooth variation of the critical indices with the corresponding electron–electron interaction constant. When evaluating the two approaches we should remember that the hypothesis of the dominant role of acoustic excitations has not been strictly justified. Furthermore, as we shall show below, the asymptotic behaviour of the pair correlation function can be inferred from the properties of the structure factor $S(k)$ at $k = 2k_F$, $4k_F$, etc., and therefore it cannot be associated with excitations of the acoustic type. On the other hand, the approach based on the linearisation of the quadratic Fermion spectrum

also has some weaknesses, the most serious of which is the inadequate symmetry of the complete wave function of the system (due to the introduction of two kinds of particle), which cannot be justified (say) by the expansion of various physical quantities in a power series of a small interaction constant.

Thus both approaches rely on plausible but not strictly justified assumptions. In our calculation[17] of the correlation functions we have developed a variant of perturbation theory which uses a non-interacting Fermi gas as the zeroth approximation, and therefore allows standard corrections to be applied to the correlation function. Our method treats a one-dimensional system of $N$ particles (whose spin is ignored to simplify the problem), distributed over the region $[0, L]$, by the continuum model of a Fermi gas, whose Hamiltonian is

$$\hat{H} = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + g \sum_{i \neq j}^{N} V(x_i - x_j) . \qquad (1)$$

Here $V(x)$ is the interaction potential, assumed to be arbitrary, and $g$ is the interaction constant. As stated above, the most serious difficulty in the calculation of the correlators is our lack of knowledge of the form of the wave functions of this system. We started from the following representation of the wave function of the ground state:

$$\Psi(x_1, \ldots, x_N) = \Psi_0(x_1, \ldots, x_N) \cdot \exp[\Phi(x_1, \ldots, x_N)] \qquad (2)$$

where $\Psi_0$ is the wave function of the system without interaction (the Slater determinant), which is antisymmetrical with respect to permutation of particle coordinates, and $\Phi(x_1, \ldots, x_N)$ is a symmetric function.

Inserting $\Psi$ into the Schrödinger equation gives an equation for $\Phi$. Since the function $\Phi$ is symmetric, the equation obtained is the Hamiltonian of the Bose particles. This "Bosonisation" of the Fermi problem has several interesting consquences, which lack of space prevents us from discussing. It is found that $\Phi$ takes the form

$$\Phi = \sum_{i,j} \Phi_2(x_i - x_j) + \sum_{i,j,l} \Phi_3(x_i - x_j, x_j - x_l) + \ldots \qquad (3)$$

i.e. it is made up of functions for two, three, etc. particles. It is also found (even more importantly) that the two-particle function $\Phi_2(x)$ plays the main role in determining the correlation properties. Furthermore, the asymptote of the correlators at large distances is given by the asymptote of the Fourier transform of $\Phi_2(x)$: the function $\sigma_2(k)$ for $k \to 0$.

Thus we have shown that detailed information on the wave function is not essential to the determination of the most important correlation properties of the system, and we have reduced the problem of obtaining the correlators to finding the asymptote of the function $\sigma_2(k)$, followed by suitable averaging. Though each of these problems is fairly difficult, they are much simpler than the initial problem. Our calculations show[18] that the asymptotic form of the function $\sigma_2(k)$ for $k \to 0$ is

$$\sigma_2(k) = \pi(c_0 - c)/2c_0|k| \qquad (4)$$

where $c$ and $c_0$ are the velocities of sound in the system having interaction and in the system having $V(x) = 0$ respectively. We note that the velocity of sound appears in the expression for the excitation energy: $\varepsilon(k) = c|k|$ for $k \to 0$. The velocity of sound determined in this way is consistent with the value obtained by thermodynamic arguments.

Now let us consider the density matrix $\rho(R)$. In order to evaluate it we developed a special graphical method[17] from which the asymptotic form of the $\rho(R)$ dependence at large distances $R$ can be obtained:

$$\rho(R) = \sin(k_F R)/(\pi R k_F)^{\varkappa}; \quad \varkappa = (c_0^2 + c^2)/2cc_0 . \qquad (5)$$

Since $c = c(g)$, the critical index $\kappa$ varies continuously as a function of $g$. This behaviour of $\kappa$ is typical of one-dimensional quantum systems. As was stated above, the Fourier transform of $\rho(R)$, i.e. the function $n(k)$, is a function of the distribution of the particles in momentum. The most interesting property of the function $n(k)$ is the absence of a discontinuity at $k = k_F$:

$$n(k) = \frac{1}{2}\{1 + \operatorname{sign}(k_F - k)|k - k_F|^{\varkappa - 1}\}; \quad \varkappa - 1 = (c - c_0)^2/2cc_0 . \qquad (6)$$

The jump in the momentum distribution of the particles is absent even when the $g$ value is so small that the one-dimensional system behaves very differently from a three-dimensional system. It has been shown[19,20] that in the three-dimensional case the jump persists for $g \neq 0$, though it is no longer equal to 1.

Qualitatively similar results were obtained by the linear model[8]. However, we should note that in the linear model the critical index $\kappa$ has a different value, and that for some types of interaction potential (in particular, in the case of a $\delta$-function potential) the linear model gives an incorrect value of $\kappa$ even for $g \to 0$.

We may now consider the other correlator: the pair correlation function $G(R, t)$ and its Fourier transform [the function $S(k, \omega)$]. This correlator is most conveniently discussed by starting with a special case: strong repulsion between the electrons. In this case the correlator of interest to us can be calculated exactly: thus the results can be compared with those of the linear model, and furthermore the form of the pair correlation function can be determined for arbitrary values of the interaction constant.

Let us examine a system defined by the Hamiltonian (1). The potential $V(x)$ which appears in it can be, for example, a power function, or it can have the form $V(x) = \exp(-\gamma|x|)$, where $\gamma^{-1}$ is the interaction radius. An exact analysis of this system for $g \to \infty$ and low enough temperatures is possible because of the well-known formation of a Wigner crystal with a lattice constant $a = 1/\rho = L/N$.[18] Introducing the new variable

$$x_n = na + \xi_n$$

and truncating the expansion of the potential energy at the term quadratic in $\xi_n$ we obtain the Hamiltonian for a system of harmonic oscillators with long-range effects, which can be reduced in the normal way to the Hamiltonian for a system of non-interacting phonons.

The spectrum of these oscillators defines the energy of the elementary excitations of the Fermi gas. These excitations (Fig. 1) are of the acoustic type at low values of the momentum ($q \to 0$):

$$\omega(q) = c|q|; \quad c = a\left(2g \sum_{n=1}^{\infty} V''(na)\, n^2\right)^{1/2} \qquad (7)$$

and are periodic, with a periodicity of $2k_F$, which is characteristic of one-dimensional systems in general.

In this limit ($g \to \infty$) the wave functions of the initial system reduce to the standard oscillator functions, and the calculation of $G(R, t)$ involves only taking the Gaussian integrals. The expression for $G(R, t)$ is quite cumbersome[18], and will not be reproduced here. We shall examine some

special cases only. For $t = 0$ and $r = 0$ the function $h(R) = G(R, 0) - \rho^2$ becomes

$$h(R) = 2\rho^2 \sum_{s=1}^{\infty} \cos(2k_F sR)\,(R\rho)^{-2\mu s^2};\ \mu = 2k_F/c \quad (8)$$

The asymptotic behaviour of this correlator for $R \to \infty$ is determined by the first term of this sum (for $s = 1$):

$$h(R) = 2\rho^2 \cos(2k_F R) \cdot (R\rho)^{-2\mu} \quad (9)$$

i.e. the critical index is $\alpha = 4k_F/c$. We note from formula (9) that at $T = 0$ the function $h(R)$ decreases with distance by a power law whose index depends on $g$. For $T \neq 0$ the function $h(R)$ decays exponentially with a correlation radius $\propto T^{-1}$.

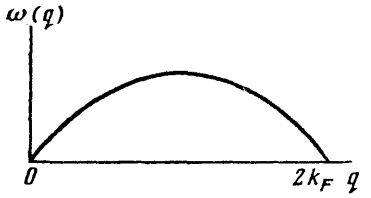



**Figure 1.** Spectrum of the elementary excitations in a one-dimensional Fermi gas.

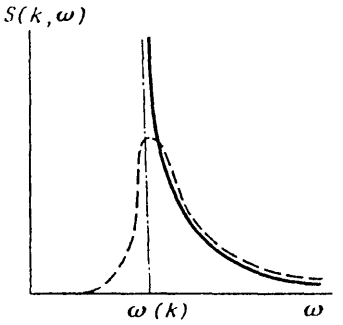



**Figure 2.** Plots of $S(k, \omega)$ against $\omega$ for a fixed $k$. The full line is for $T = 0$, the broken line for $T \neq 0$.

The following remarks are relevant in connection with the formula for $h(R)$. As stated above, the correlator $h(R)$ has been calculated exactly for some special forms of the potential $V(x)$ and some special values of $g$ (in particular, for the $V(x) = x^{-2}$ potential, used in the Sutherland model[21-24]). The velocity of sound $c$ is also known for these special cases. By inserting these values of $c$ into formula (9) for $h(R)$ we obtain good agreement with all the known exact values. Furthermore, $h(R)$ can be calculated in the limit of small $g$ by the method which we used to calculate the density matrix: comparison of the results[19] shows that the formula for $h(R)$ is valid in this case also. These observations suggest that the expression for $h(R)$ can be used for all $g > 0$ and $T = 0$ if an exact value of the velocity of sound is available for the parameter $c$ which appears in the expression.

Thus the asymptotic behaviour of both $h(R)$ and $\rho(R)$ is known if the velocity of sound $c$ is known. The problem of calculating $c$ is much simpler than the calculation of the correlator, since $c$ is effectively one of the energy parameters of the system, which can be calculated by well tried approximations. For some of the models the $c$ value is accurately known. As $g$ varies from 0 to $\infty$ the parameter $\alpha$ varies from 2 to 0. It is interesting to compare the expression for $h(R)$ with the corresponding expression of the linear model. The latter also gives a power-law decrease in the correlator as $R \to \infty$, but with a different exponent, except at low values of $g$.

The Fourier transform of $G(R, t)$—the dynamic structure factor $S(k, \omega)$—defines the probability of scattering neutrons and X-rays. The plot of $S(k, \omega)$ against $\omega$ (Fig.2) for a fixed value of $k$ shows a singularity at $\omega \to \omega(k)$ for all $g > 0$ and fixed $k$ ($S(k, \omega)_{g=0} = \text{const.}$), described by a power law with the exponent $1 - \alpha/2$. For $T \neq 0$ this singularity is smoothed out, and a maximum appears in $S(k, \omega)$ at $\omega = \omega(k)$ (broken line in Fig.2).

It is interesting also to consider the correlator $S(k)$, i.e. the static structure factor which determines the probability of elastic scattering of X-rays and is the Fourier transform of the correlator $h(R)$.

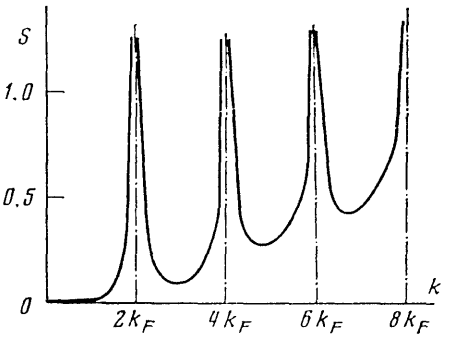



**Figure 3.** $S(k)$ dependence in the Sutherland model for $g = 2 \times 10^4$ and $T = 0$.[18]

Figs.3 and 4 show plots of the function $S(k)$ at $T = 0$ and at $T \neq 0$ for different values of $g$ in the Sutherland model. At $T = 0$ the function $S(k)$ is discontinuous at the $k$ values $k \to 2k_F n$, and we can write $S(k) = |k - 2k_F n|^{\alpha n^2 - 1}$. The number of peaks, i.e. the number of points $n$ at which the function diverges, satisfies the condition $c > 4k_F n^2$, and therefore the number of peaks increases with $g$. We also note that the leading term of the asymptote of the function $h(R)$ is determined by the singularity in $S(k)$ at $k = 2k_F$. The effects at $k = \pm 4k_F$, $\pm 6k_F$, etc. correspond to the further terms of the expansion ($s = 2$, 3, etc.) in formula (8). We should note that the singularities of the function $S(k)$ at $k = \pm 2k_F n$ (with $n \geq 2$) are "lost" in the linear model. At $T \neq 0$ the discontinuities in the function $S(k)$ are rounded off, and the value of $S(k)$ is finite for all $k$, with

$$S(0) = 2k_B T/c^2;\quad S(2k_F n) = \coth(2\pi^2 n^2 k_B T/c^2) \quad (10)$$

As the temperature is raised the height of the peaks decreases. It can be shown that the function $S(k)$ plotted in Fig.4 is valid not only at low temperatures (to which our

discussion applies) but even in the high temperature limit, where the classical approximation can be used. It was found[25,26] that the function $S(k)$ has maxima at $k = 2k_F n$, and the height of the peaks decreases as $n$ increases. These calculations were intended to explain experimental data[26] on the diffuse scattering of X-rays by linear chains of mercury atoms in the quasi-one-dimensional $Hg_{3-\delta}AsF_6$ system. The $S(k)$ dependence obtained experimentally is similar to that shown in Fig.4 and agrees well with the calculations[25,26]. It follows from the expressions for $h(R)$ and $S(k)$ that an interacting Fermi gas is structurally closer to a one-dimensional solid than to a liquid.

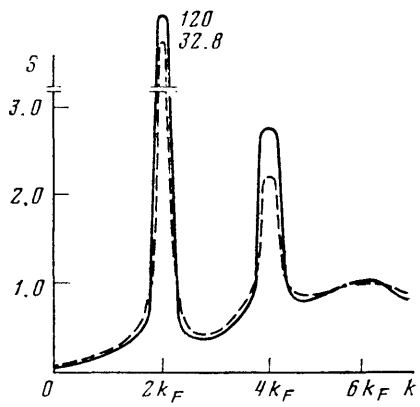



**Figure 4.** $S(k)$ dependence in the Sutherland model for $g = 200$. Full line $k_B T/\rho^2 = 3/5$; broken line $k_B T/\rho^2 = 3$. The numbers on the curves denote the height of the peak at $k = 2k_F$.[18]

The main conclusions from the above discussion of the correlators for a one-dimensional interacting Fermi gas can be formulated as follows. At large distances and $T = 0$ the correlation functions decrease by a power law, with an exponent expressed simply in terms of the velocity of sound. Reliable methods of calculating the velocity of sound are available, and for some models this parameter is already accurately known. Both methods of calculating the correlators (by linearising the problem or by postulating predominantly acoustic excitation in the formulation of the special features of the correlators) give functionally correct predictions of the asymptotes of the correlators, but the critical exponents are correctly calculated only for small $g$: evidently, the linearisation procedure as described is valid only in this region of $g$ values.

A new approach to the calculation of correlators has been proposed recently by Haldane[27], who used assumptions basically similar to those of Ref.13 to convert the problem into an oscillator problem and obtained experessions for the correlators identical to ours.

## III. LATTICE FERMI GAS

So far our discussion has been confined to the continuum model of a one-dimensional Fermi gas. A more realistic model of the system is provided by the lattice Fermi gas, which describes a system of $N$ interacting electrons located at $M$ centres, with $N \to \infty$ and $M \to \infty$ and $N/M = \rho$. The continuum and the lattice model have a great deal in common both from the electronic structure and from the correlator point of view. Thus, the correlator $\rho(R)$ for the lattice Fermi gas can be calculated as in the continuum case, the steps in the Fermi distribution becomes diffuse[28] however weak the interaction, with a critical index $\kappa$ for $g \ll 1$ given by

$$\kappa = 1 + g^2 v^2(0)/32\pi^2\beta^2 \sin^2(\pi\rho/2)$$

where $v(q)$ is the Fourier transform of the function $V(x)$ [$v(0) = v(q = 0)$, and $\beta$ is the resonance integral].

At the same time, lattice systems offer a number of special features. For example, in contrast to continuum models (for which the elementary excitation spectrum has no gap) the lattice systems can have a gap. Lastly, for stated values of the parameters the lattice systems allow long-range order at $T = 0$.

Let us consider the simplest (but by no means trivial) lattice model: a Fermi gas without spins and with interactions between nearest neighbours. Its Hamiltonian is

$$\hat{H} = -\beta \sum_{n=1}^{N} (a_n^+ a_{n+1} + a_{n+1}^+ a_n) + g \sum_{n=1}^{N} a_n^+ a_n a_{n+1}^+ a_{n+1}; \ \rho = 1/2; \ g > 0 \quad (11)$$

where $a_n^+$ and $a_n$ are operators for the generation and annihilation of Fermions on the $n$th centre. This system is interesting also because it is equivalent to the anisotropic antiferromagnetic Heisenberg model. Mathematically, the term "equivalent" postulates the existence of a canonical transformation[29] which converts the Fermi operators into spin operators, so that Eqn.(11) reduces to the Hamiltonian of the Heisenberg model.

An interesting property of this system is the presence of a gap in the elementary excitation spectrum for $g > 2\beta$.[30,31] In this range of $g$ values the system displays long-range order, i.e. the correlator $h(R)$ tends towards a finite limit determined by the ratio $g/\beta$ at $R \to \infty$. In magnetic systems this implies the existence of non-zero magnetisation of the sublattices. The asymptote of $h(R)$ differs from its limiting value, first calculated by Baxter[32], by an exponentially small quantity. For $g < 2\beta$ the spectrum of the system no longer has a gap, and the long-range order disappears[30,31]. If controlled changes in $\beta$ (say) are imposed on the system a metal $\to$ dielectric transition is obtained at $\beta = g/2$, when both the gap and the long-range order disappear.

Unfortunately, no strict calculations of pair correlation functions in a metallic phase have been reported yet, and only approximate expressions for this correlatore are so far available. They were obtained[33-35] from the following considerations. The spectrum of elementary excitations of the system is of the form shown in Fig.5.[36] The cross-hatched region is called the two-parameter continuum; its upper and lower limits are the $\varepsilon_2(k)$ and $\varepsilon_1(k)$ curves, given (for $g = 2\beta$, for example) by the expressions

$$\varepsilon_2(k) = \pi g |\sin(k/2)|; \ \varepsilon_1(k) = (\pi g/2)|\sin k|.$$

Against each triangle in Fig.5 is shown the value of $S(k, \omega)$ for the corresponding $k$ and $\omega$ obtained[33] in calculations for systems with a finite number of electrons $N = 10$. These calculations show that for the states lying above the two-parameter continuum the $S(k, \omega)$ values are at least an order of magnitude smaller than for the states within the continuum. Assuming that even at $N \to \infty$ the higher states do not contribute significantly, the following expression for $S(k, \omega)$

was obtained[33]

$$S(k,\ \omega) = A\theta[\omega - \varepsilon_1(k)]\,\theta[\varepsilon_2(k) - \omega]\cdot[\omega^2 - \varepsilon_1^2(k)]^{-\lambda_1}\,[\varepsilon_2^2(k) - \omega^2]^{-\lambda_2}$$

$$\theta(x) = \begin{cases} 1, & x > 1 \\ 0, & x \leqslant 0 \end{cases},$$

where $A$ is a constant, and the exponents $\lambda_1$ and $\lambda_2$ are chosen in relation to known constraints (for example, for $g = 2\beta$, $\lambda_1 = 1/2$ and $\lambda_2 = 0$). The approximate expression for $S(k, \omega)$ thus obtained is functionally similar to the corresponding expression of the continuum model, confirming the similarity between the continuum and the lattice model in the metallic phase.

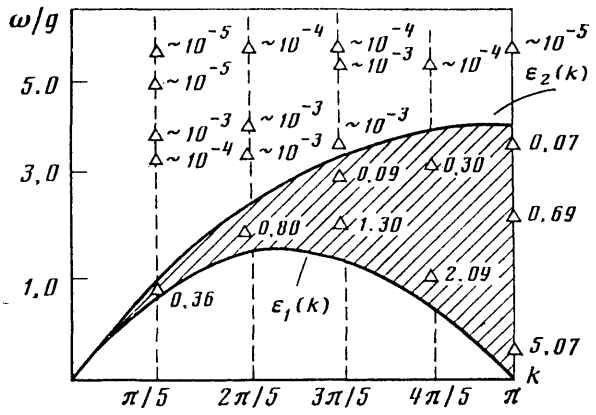



**Figure 5.** Excitation spectrum of a lattice Fermi gas and $S(k, \omega)$ values for $N = 10$.[33]

## IV. EXAMPLES OF THE USE OF CORRELATION FUNCTIONS

We shall illustrate the above discussion by giving two examples of the use of correlation functions: 1) to interpret experimental data on the inelastic scattering of neutrons by a one-dimensional system, and 2) to calculate the critical phase transition temperatures in quasi-one-dimensional systems.

1) The most meaningful experiments on the inelastic scattering of neutrons by one-dimensional systems of the present type were carried out with the one-dimensional antiferromagnetic CPC $[CuCl_2.2N(C_5D_5)]$.[37,38] As was stated above, a one-dimensional antiferromagnetic is equivalent to a one-dimensional lattice Fermi gas with repulsions between particles. Experimental data on the inelastic neutron scattering cross-section of CPC are reproduced in Fig.6*a*. We note that the asymmetry of the line and the intensity at the maximum increase as the temperature is lowered. The asymmetry was initially thought[37] to be an apparatus effect, but its reality was confirmed by later experiments[38]. The effect is easily explained in terms of the temperature dependence of $S(k, \omega)$, theoretically predicted (see Fig.2) and arising from the properties of the function $S(k, \omega)$ at $\omega = \omega(k)$.

The integral scattering intensity experimentally observed at $T = 1.3$ K (Fig.6*b*) suggests a singularity in $S(k)$ at $k \to 2k_F$ (in this case $k_F = \pi/2$) and agrees very well with the theoretical expression given by Müller[33].

2) The calculation of the critical transition temperature in quasi-one-dimensional systems. As we have already stated, long-range order is absent in one-dimensional systems at $T \neq 0$ (though it can exist at $T = 0$ in the lattice systems discussed above). In real systems a small but significant lateral interaction between the one-dimensional systems (filaments) is always present. As a result, at low enough temperatures the one-dimensional systems becomes effectively three-dimensional, and they develop long-range order (which disappears at $T = T_{cr}$).

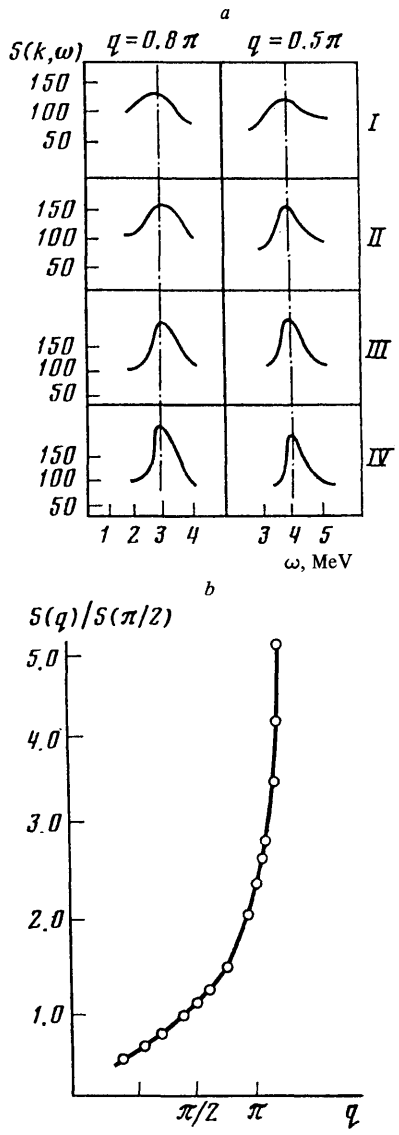



**Figure 6.** (*a*) Inelastic neutron scattering cross-section for CPC in relative units for two values of $q$, and (*b*) integral scattering intensity, for different temperatures ($T$): *I*) 8.0, *II*) 4.0, *III*) 2.0, *IV*) 1.3 K.[37,38]

We shall illustrate the calculation of $T_{cr}$ from a knowledge of the one-dimensional correlators by considering the trivial but very revealing example[39] of a two-dimensional system of

ferromagnetic Eising chains with weak transverse interactions. The Hamiltonian of this system is

$$\hat{H} = -J_{\parallel} \sum_{i,m} S^z_{i,m} S^z_{i+1,m} - J_{\perp} \sum_{i,m} S^z_{i,m} S^z_{i,m+1};\ J_{\parallel} > 0;\ J_{\perp} > 0\ , \quad (12)$$

where $J_{\parallel}$ and $J_{\perp}$ are the exchange integrals for the interaction of nearest neighbours along chains and at right angles to the chains respectively, and $S^z_{i,m}$ is the operator for the $z$-component of the spin at the lattice point numbered $(i, m)$.

We shall use the self-consistent field approximation and replace one of the operators in the second term by its average value $\langle S^z \rangle$:

$$\hat{H} = -J_{\parallel} \sum_{i,m} S^z_{i,m} S^z_{i+1,m} - 2J_{\perp} \langle S^z \rangle \sum_{i,m} S^z_{i,m}\ , \quad (13)$$

with the self-consistence condition

$$\langle S^z \rangle = \mathrm{Sp}\, S^z_{i,m} \exp(-\hat{H}/k_B T) / \mathrm{Sp} \exp(-\hat{H}/k_B T)\ . \quad (14)$$

At $T \to T_{cr}$ we have $\langle S^z \rangle \to 0$, and by expanding the right-hand side of (15) into a power series in $\langle S^z \rangle$ we obtain the following expression for calculating $T_{cr}$:

$$k_B T_{cr} = 2J_{\perp} \sum_n \langle S^z_0 S^z_n \rangle\ . \quad (15)$$

The one-dimensional correlation function $\langle S^z_0 S^z_n \rangle$ appears in this expression. Thus, knowing the one-dimensional correlator $\langle S^z_0 S^z_n \rangle = \tanh^n |(J_{\parallel}/4k_B T)/4$, we can calculate $T_{cr}$ by solving Eqn.(15):

$$k_B T_{cr} = 2J_{\parallel} / \ln (J_{\parallel}/J_{\perp})\ .$$

The exact value of $T_{cr}$, obtained by solving Onsager's equation, is given by

$$k_B T_{cr} = 2J_{\parallel} / \ln (2J_{\parallel}/J_{\perp})\ .$$

These calculations can easily be generalised to include more complex systems[13,40,41]. For example, we can use exactly the same arguments to calculate $T_{cr}$ for a three-dimensional lattice gas with weak transverse interactions[41]:

$$\hat{H} = \hat{H}_0 + \hat{H}_1;\ \hat{H}_0 = -\beta \sum_{i,m} (a^+_{i,m} a_{i+1,m} + a^+_{i+1,m} a_{i,m}) +$$
$$+ g_{\parallel} \sum_{i,m} a^+_{i,m} a_{i,m} a^+_{i+1,m} a_{i+1,m};\quad \hat{H}_1 = g_{\perp} \sum_{i,m} a^+_{i,m} a_{i,m} a^+_{i,m+1} a_{i,m+1}\ .$$

The subscript $i$ gives the number of the site along the filament, whereas $m$ defines the site in the perpendicular direction. For $T < T_{cr}$ we have a long-range order phase (called the phase with a charge density wave), in which three-dimensional effects appear, whereas for $T > T_{cr}$ the system is essentially one-dimensional.

Using the self-consistent field approximation and inserting the self-consistence condition we arrive at the equation

$$1 = 2v \int_0^{(k_B T_{cr})^{-1}} d\tau \sum_n (-1)^n G(n, \tau)\ ,$$

where $\nu$ is the number of nearest filaments, and $G(n, \tau)$ is the one-dimensional pair correlation function for imaginary time. As in the previous example we must know the purely one-dimensional correlation function in order to determine $T_{cr}$. The equation for $T_{cr}$ is more complex than that given by the Eising model because $H_0$ and $H_1$ are not commutable in this model (in contrast to the Eising model). The parameter $T_{cr}$ is given by the above equation as

$$k_B T_{cr} = C g_{\perp};\ C \sim 1\ .$$

It is interesting to compare the two models in the light of the fact that the Eising model is the limiting case of the lattice model for $g \gg \beta$, i.e. it aims to model the lattice Fermi gas in the dielectric phase (at $T = 0$) which was discussed above. Thus the two examples considered here describe the three-dimensional ordering of filaments in dielectric or in metallic phases (at $T = 0$). From the corresponding expressions for $T_{cr}$ we note that the transition temperature is substantially higher for filaments in the dielectric phase.

We should stress that the self-consistent method described above can also be used to find approximate expressions for the quasi-one-dimensional correlation functions in an ordered (three-dimensional) phase.

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