Correlation functions in one-dimensional systems with a strong interaction

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The correlation functions are found for a one-dimensional Fermi gas with an infinitely strong attraction. It is shown that acoustic excitations make the major contribution to the forming of the singularities of the correlation functions. The hypothesis is expressed that acoustic excitations are also essential in the case of an arbitrary attraction. On the basis of this hypothesis, the form of the correlation functions is derived for arbitrary attraction. The obtained results are applied to a one-dimensional Bose gas with repulsion. The effects of the quasi-one-dimensional nature of the problem, which lead to dielectric or superconducting transitions, are considered.

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INTRODUCTION

There are no phase transitions in one-dimensional systems, and at finite temperatures there is no long-range order. However, at low temperatures the correlation functions decrease slowly with distance. The law governing this decrease determines the superconducting transition temperature in quasi-one-dimensional systems[1] and is of independent interest.

In the one-dimensional case, the correlation functions have been found in several models: in a model having a large number of bands[1] and in models having a linear spectrum.[2-4] In all of these models the correlation functions at zero temperature fall off with distance according to a power law, as $R^{-\alpha}$. In more realistic models with a short-range potential characterizing the interaction between the particles, the exact solution has been found for the wave function and for the energy of the ground state,[5] but the form of the correlation functions is unknown. Approximate methods exist for the case of a weak interaction between the electrons, these methods being based on a summation of "parquet" diagrams or on the utilization of the renormalization group. These methods are not applicable at low temperatures, when the interaction ceases to be weak.

We consider below the opposite limiting case, when a strong attraction exists between the electrons and the binding energy of two electrons is much larger than the Fermi energy. Such a model is equivalent to the model of a Bose gas with infinitely strong repulsion. The thermodynamics of this Bose gas coincides with the thermodynamics of spinless fermions. The single-particle correlation functions of the bosons are expressed in terms of Toeplitz determinants. At low temperatures the correlation functions fall off at large distances according to an exponential law, with the correlation radius being inversely proportional to the temperature. At zero temperature the single-boson correlation function falls off with distance according to a power-law with the exponent equal to 1/2. For an arbitrary attraction between the electrons, the form of the correlation functions at large distances is determined by acoustic vibrations. These oscillations destroy the long-range order at zero temperature. In this case the pair correlation function G(R) and the density correlation function Π(R) fall off according to the laws

$$G(R)\sim R^{-\alpha}, \quad \Pi(R)\sim\cos(2p_FR)R^{-1/\alpha}.$$

The value of the exponent α depends on the interaction between the electrons. $\alpha = 1/2$ for the case of strong attraction, and $\alpha = 1$ for weak attraction. It is likely that spin waves play the role of acoustic excitations in the case of repulsion for a half-filled band.

The form of the pair correlation function in the one-dimensional case enables one to estimate the superconducting transition temperature in a quasi-one-dimensional metal, which has a power-law dependence on the probability of electron hopping from filament to filament. The interaction between the electrons on different filaments may lead to a transition into a dielectric state.

1. REDUCTION OF THE PROBLEM TO AN IDEAL FERMI GAS

The interelectron attraction via the a phonon or non-phonon mechanism is usually assumed to be weak. In real quasi-one-dimensional systems such an attraction may turn out to be large. Therefore, the case of strong interaction is of interest. Below we shall assume that the binding energy of two electrons, which are located on a single molecule, is larger than the width of the band. The Hamiltonian of such a system has the form

$$H=I\sum_{i,\alpha}a_{i,\alpha}^{+}(a_{i+1,\alpha}+a_{i-1,\alpha})-V\sum_{i,\alpha}a_{i,\alpha}^{+}a_{i,-\alpha}^{+}a_{i,-\alpha}a_{i,\alpha}-\sum_{i\neq j,\alpha,\beta}V_{ij}a_{i\alpha}^{+}a_{j\beta}^{+}a_{j\beta}a_{i\alpha}, \tag{1}$$

where $a_i^+(a_i)$ are the electron creation (annihilation) operators, and I denotes the width of the band. The subscripts i and α denote the site labels and the spin-states of the electrons.

All of the electrons are bound in pairs in the limiting case V ≫ I. At each lattice site there are either two electrons with opposing spins or else no electrons at all. The states with one electron per site are separated by a large gap, equal to V. If these states are not taken into consideration, the operators describing the creation (or annihilation) of a pair of electrons

$$b_i^{+}=a_{i,+}^{+}a_{i,-}^{+}, \quad b_i=a_{i,-}a_{i,+} \tag{2}$$

satisfy the following commutation relations:

$$b_i^{+}b_j-b_jb_i^{+}=0, \quad i\neq j, \quad b_i^{+}b_i+b_ib_i^{+}=1, \quad b_ib_i=b_i^{+}b_i^{+}=0. \tag{3}$$

The density operator ρ_i of the electrons is given by

$$\rho_i=\sum_{\sigma}a_{i,\sigma}^{+}a_{i,\sigma}=2b_i^{+}b_i. \tag{3a}$$

In second order with respect to the overlap integral

I, the Hamiltonian (1) can be expressed in terms of the operators b_i:

$$H=\frac{1}{2m}\sum_i b_i^+(b_{i+1}+b_{i-1})+\sum_{i\neq j}\rho_i\rho_j\left[\frac{1}{8m}\delta(|i-j|-1)-V_{ij}\right]-2V\sum_i b_i^+b_i, \tag{4}$$

where $1/2m = I^2V$. The case

$$V_{ij}=\frac{1}{8m}\delta(|i-j|-1) \tag{4a}$$

will be investigated below. For such a choice of the interaction V_{ij}, the problem has an exact solution, and in the following sections this exact solution is utilized in order to verify the hypothesis that enables us to find the correlation functions for an arbitrary interaction.

The Hamiltonian (4) and the conditions (3) and (4a) describe a boson gas with an infinite repulsion between bosons located at a single point. The wave functions of such a system were first determined by Girardeau.[6] The thermodynamics of such a gas coincides with the thermodynamics of an ideal gas of spinless fermions. We shall be interested in the correlation function $G(R) = \langle b_i^+ b_R\rangle$. Just as in the case of the XY-model of a one-dimensional ferromagnetic substance,[7] let us change to spinless fermion operators

$$b_i=\prod_{j<i}(1-2c_j^+c_j)c_i, \qquad b_i^+=c_i^+\prod_{j<i}(1-2c_j^+c_j). \tag{5}$$

One can easily verify that, for the usual commutation relations between the Fermi operators c_i, the relations (3) are fulfilled for the operators b_i. The Hamiltonian (4) is expressed in terms of the operators c_i in the following way:

$$H-\mu N=\frac{1}{2m}\sum_i\left[c_i^+(c_{i+1}+c_{i-1})-\mu c_i^+c_i\right]=\frac{L}{2\pi}\int_0^{2\pi}\varepsilon_p c_p^+c_p\,dp, \tag{6}$$

where $\epsilon_p = -m^{-1}\cos p - \mu$, L is the length of the sample, and μ is the chemical potential. The last term in formula (4) is included in the chemical potential.

2. THE PAIR CORRELATION FUNCTION

With the aid of formula (2) the pair correlation function G describing the superconducting fluctuations can be expressed in terms of the single-boson correlation function:

$$G(R)=\langle a_{0,+}^+a_{0,-}^+a_{R,-}a_{R,+}\rangle=\langle b_0^+b_R\rangle.$$

Expressing the boson operators in terms of the spinless fermion operators c and c^+, we obtain

$$G(R)=\left\langle c_0^+\prod_{1<m<R}(2c_m^+c_m-1)c_R\right\rangle. \tag{7}$$

According to Wick's theorem, the average of the product can be expressed in terms of the product of the averages:

$$G(R)=\mathrm{Det}\,(g_{n,\,m+1}), \tag{8}$$

where

$$g_{nm}=2\langle c_n^+c_m\rangle-\delta_{nm}=\int_0^{2\pi}\frac{dp}{2\pi}g_p e^{ip(n-m)}, \qquad g_p=\mathrm{th}\frac{\varepsilon_p}{2T}. \tag{9}$$

In formula (8) n and m take values from 0 to R − 1. The matrix elements G_{nm} only depend on the difference n − m. Therefore, the determinant in expression (8) is a Toeplitz determinant. In the asymptotic region $R\to\infty$ the behavior of this determinant is determined by the Szegö formula:[8]

$$G(R)=\exp\left[K_0R+\sum_{n=1}^{\infty}nK_nK_{-n}\right], \tag{10}$$

where

$$K_n=\int_0^{2\pi}\frac{dp}{2\pi}e^{inp}\ln\left(e^{-ip}\,\mathrm{th}\frac{\varepsilon_p}{2T}\right). \tag{11}$$

At low temperatures $T \ll \mu$ the integral (11) is given by

$$K_n=\begin{cases}\dfrac{(-1)^n}{n}\dfrac{e^{ip_0n}}{1+e^{-n\pi Tm/\sin p_0}} & \text{for } n\neq 0\\ -\pi Tm/2\sin p_0 & \text{for } n=0\end{cases} \tag{12}$$

where p_0 is the Fermi momentum ($-\cos p_0 = m\mu$). Substituting expression (12) in formula (10), we obtain

$$G(R)=A(mT)^{1/4}e^{-\pi TRm/2\sin p_0}. \tag{13}$$

Here

$$\ln A=-2\int_0^{\infty}\frac{e^{-t}}{t}\left[\frac{1}{(1+e^{-t})^2}-\frac{1}{4}\right]dt+\ln 2\pi-\frac{3}{2}C,$$

and C is Euler's constant. Formula (13) is valid in the asymptotic region $mTR \gg \sin p_0$.

It is shown in the Appendix that the correlation function has the following scaling form at low temperatures and over large distances:

$$G(R)=R^{-\alpha}f(mTR/\sin p_0). \tag{14}$$

Comparison with expression (13) allows us to reach the conclusion that $\alpha = 1/2$ and the correlation function at T = 0 behaves like

$$G(R)\propto R^{-1/2}. \tag{15}$$

Thus, Bose condensation (long-range order) is absent even at T = 0, but the correlation function falls off with distance according to a power law, and not exponentially as it does at finite temperatures.

3. CORRELATION OF THE DENSITIES

Let us now proceed to an evaluation of the density correlation function

$$\Pi(R,t)=\langle\rho_{0,0}\rho_{R,t}\rangle-\bar{\rho}^2, \tag{16}$$

where ρ is determined by formula (3a). It follows from formula (5) that $b_m^+b_m = c_m^+c_m$. Therefore, the density correlation function (16) coincides with the density correlation function for an ideal gas of spinless fermions. The Fourier component $\Pi(q,\omega)$ of this correlation function is given by

$$\Pi(q,\omega)=-2\int\frac{\mathrm{th}[\varepsilon(p)/2T]-\mathrm{th}[\varepsilon(p-q)/2T]}{\omega-\varepsilon(p)+\varepsilon(p-q)}\frac{dp}{2\pi}. \tag{17}$$

For small values of q and ω, the Fourier component $\Pi(q,\omega)$ is of the form

$$\Pi(q,\omega)=-\frac{4}{\pi}\frac{q^2v}{\omega^2-v^2q^2}, \tag{18}$$

where $v = \partial\epsilon/\partial p$ denotes the velocity at the Fermi surface.

It is obvious from formula (18) that acoustic excitations exist in the system. The speed of sound is expressed in terms of the compressibility in the usual way. For values of q close to $2p_0$ and small values of ω, the polarization operator $\Pi(q,\omega)$ has a logarithmic singularity:

$$\Pi(q,\omega)=\frac{2}{\pi v}\ln\frac{\mu}{\max\{\omega,|q-2p_0|,T\}}. \tag{19}$$

The probabilities for the scattering of neutrons and x rays are determined by the imaginary part of the correlation function $\Pi(q,\omega)$. For values of the momentum transfer close to $2p_0$, the scattering probability is proportional to

$$\frac{1}{v}e^{\omega/2T}\left[\operatorname{ch}\frac{\omega+v(q-2p_0)}{4T}\operatorname{ch}\frac{\omega-v(q-2p_0)}{4T}\right]^{-1}. \quad (19a)$$

At coincident times and at low temperatures we obtain

$$\Pi(R,0)=\frac{T^2\sin^2 p_0R}{v^2\operatorname{sh}^2(\pi TR/v)}. \quad (20)$$

This formula indicates that there is no long-range order even at zero temperature, and there is no transition into a dielectric state (Peierls transition). At finite temperatures the correlation function falls off exponentially. An exponential decrease of the correlation function was predicted in [9]; however, as is clear from formula (20), the correlation length varies in inverse proportion to the temperature. Evidently this means that a model with the true order parameter,[9] which leads to an exponential dependence of the correlation length on the temperature at low temperatures, describes the density correlation function poorly when the momentum is close to $2p_0$. Furthermore, the small pre-exponential factor T^2 appears in formula (20), and at distances smaller than the correlation length the correlation function decreases in inverse proportion to the square of the distance, just as at zero temperature. As is shown below, the power-law behavior of the correlation functions is related to the quantum nature of the fluctuations and cannot be obtained by the classical methods applied in [10,11].

4. THE ROLE OF THE ACOUSTIC EXCITATIONS IN FORMING THE SINGULARITIES OF THE CORRELATION FUNCTIONS

The exact results obtained above enable us to verify the hypothesis that, in one-dimensional systems the behavior of the correlation functions at large distances and low temperatures is determined by the acoustic excitations. In the model under consideration this hypothesis allows us to obtain the general form of the correlation functions, which agrees with the exact solution in all cases where this solution is known. In the model with a large number of conducting bands,[1] such an hypothesis has been rigorously justified. The behavior of the correlation functions was determined by the long-wavelength gapless excitations. The contribution of the other excitations was small. In the case of a single conducting band, this contribution was not small, but apparently only leads to the appearance in the correlation functions of factors which are independent of the temperature and of the coordinates.

The long-wavelength gapless excitations are described by the Hamiltonian

$$\hat{H}=\frac{1}{2}\int\left[\frac{(\hat{\rho}(x)-\bar{\rho})^2}{K}+Kv_s^2\left(\frac{\partial\hat{\varphi}(x)}{\partial x}\right)^2\right]dx, \quad (21)$$

where $K=\delta\bar{\rho}/\sigma\mu$ is the compressibility and v_S is the speed of sound. The density and phase operators, $\hat{\rho}(x)$ and $\hat{\varphi}(x)$, satisfy the following commutation relation:

$$[\hat{\rho}(x)\hat{\varphi}(x')]=\delta(x-x'). \quad (22)$$

As is clear from expression (18), in the model considered in the preceding sections we have

$$K=4/\pi v, \quad v_s=v=\sin p_0/m. \quad (23)$$

The single-boson correlation function is given by

$$G(R,\tau)\sim\bar{\rho}\langle T_\tau\exp\{2i(\hat{\varphi}(R,\tau)-\hat{\varphi}(0,0))\}\rangle, \quad (24)$$

where T_τ is the time-ordering operator, and τ is the "imaginary" time. The averaging in expression (24) is carried out over the Gibbs distribution with the Hamiltonian (21). By using the Feynman method,[12] the calculation of the average in expression (24) can be reduced to an evaluation of the following path integral:

$$G(R,\tau)\sim\bar{\rho}\left(\int e^{-F[\varphi]}D\varphi\right)^{-1}\int e^{i\varphi(R,\tau)-i\varphi(0,0)}e^{-F[\varphi]}D\varphi, \quad (25)$$

where the functional $F[\varphi]$ is given by

$$F[\varphi]=\frac{K}{2}\int\left[\left(\frac{\partial\varphi}{\partial\tau}\right)^2+v_s^2\left(\frac{\partial\varphi}{\partial x}\right)^2\right]dx\,d\tau. \quad (26)$$

Evaluating the Gaussian integrals in (25), we obtain

$$G(R,\tau)=A(mT)^\alpha\exp\left\{-\frac{\pi TR\alpha}{v_s}\right\}\left|1-\exp\left\{-2\pi T\left(\frac{R}{v_s}+i\tau\right)\right\}\right|^{-\alpha} \quad (27)$$

where

$$\alpha=2(\pi Kv_s)^{-1}, \quad (27a)$$

A is a number of the order of unity, determined by the short wavelength fluctuations. At coincident moments of time we have

$$G(R,0)=A\left(mT\Big/\operatorname{sh}\frac{\pi RT}{v_s}\right)^\alpha. \quad (28)$$

At large distances $RT/v_S \gg 1$ expression (28) coincides with expression (13), obtained with the aid of the Szegö formula, if it is assumed that the coefficient A is the same as in (13) but K and v_S are taken from formula (23). The next three terms of the expansion with respect to $\exp(-RT/v_S)$ are found in the Appendix and agree with the corresponding expansion in expression (28).

Now let us calculate the effect of the acoustic excitations on the form of the density correlation function when the momentum is close to $2p_0$. Short-range order exists over small distances, and the density contains a term $\tilde{\rho}$ proportional to $\cos 2p_0x$. In connection with a slow variation of the average density, the Fermi momentum p_0 is determined by the local value of the average density, so that

$$\tilde{\rho}(x)=\bar{\rho}\cos[2p_0x+\theta(x,\tau)], \quad \frac{\partial\theta}{\partial x}=\pi(\rho-\bar{\rho}). \quad (29)$$

Slow, acoustic fluctuations of the density $\rho(x)$ lead to the disappearance of the long-range order. The density correlation function is given by

$$\tilde{\Pi}(R,\tau)\langle\tilde{\rho}(0,0)\tilde{\rho}(R,\tau)\rangle\sim\bar{\rho}^2\cos 2p_0R\,\langle\exp\{i[\theta(R,\tau)-\theta(0,0)]\}\rangle. \quad (30)$$

If the operator $\hat{I}=\nabla\hat{\varphi}/\pi$ is introduced instead of the operator $\hat{\varphi}$, such that the commutation relation $[I(x), \theta(x')] = \delta(x-x')$ is satisfied, then in terms of the new notation the Hamiltonian (21) has the form

$$\hat{H}=\frac{1}{2}\int\left[\pi^2Kv_s^2\hat{I}^2+\frac{(\nabla\hat{\theta})^2}{\pi^2K}\right]dx. \quad (31)$$

The calculation of the average in formula (30) agrees with the calculation in formula (24) after the replacement $K^{-1}\to\pi^2Kv_S^2$. Having made such a substitution in formula (27), we obtain

$$\tilde{\Pi}(R,\tau)=\frac{1}{2}\left(\frac{\gamma T}{v}\right)^{1/\alpha}\cos 2p_0R\times\exp\left(-\frac{\pi RT}{v_s\alpha}\right)\left|1-\exp\left\{-2\pi T\left(\frac{R}{v_s}+i\tau\right)\right\}\right|^{-1/\alpha} \quad (32)$$

where α is determined by formula (27a). The numerical coefficient in formula (32), arising from the short wavelength fluctuations, is chosen such that this formula (32) would coincide with the oscillating part of expressions (17), (19), and (20) if K and v_S are taken from formulas (23).

The hypothesis concerning the role of the acoustic excitations allows us to believe that formulas (27) and

(32) are valid for arbitrary attraction between the electrons. However, the exponents generally depend on the interaction. For example, for a small number of carriers in the band, when the spectrum is quadratic, the coefficient associated with $(\nabla\varphi)^2$ in the Hamiltonian (21) does not depend on the interaction and is equal to the average density. The compressibility and, therefore, the coefficient $K = \partial\bar{\rho}/\partial\mu$ depend on the interaction and vary by four times from the value (23) associated with strong attraction up to the value $K = 1/\pi v$ for an almost perfect Fermi gas. In this connection the exponents in formulas (27) and (32) change by a factor of two, so that $G \sim \Pi \sim R^{-1}$.

From an analysis of the exact solutions, one can conclude[13,14] that gapless, acoustic excitations exist at any interaction. The Coulomb interaction merits special investigation due to its long-range nature. In the case of a single filament, this interaction leads to a logarithmic divergence of the coefficient K. However, in real quasi-one-dimensional systems of parallel filaments, the Coulomb interaction is screened and, as is shown in [1], this effectively amounts to increasing the coefficient K^{-1} by the amount $e^2 \ln p_0 d$, where d is the distance between the filaments. Thus, just as in the case of arbitrary repulsion, the Coulomb interaction leads to a more rapid decrease of the superconducting correlation functions G with distance and a slower decrease of the dielectric correlation functions Π.

Formulas (13), (15), and (20) correctly describe the behavior of the correlation functions for a Bose gas with infinite repulsion. It is clear from the exact solution (15) that acoustic excitations exist for any arbitrary repulsion. The hypothesis concerning the role of the acoustic excitations permits us to believe that formulas (27) and (32) are valid for arbitrary repulsion between the bosons. Only the exponent α appearing in these formulas depends on the strength of the interaction. In the limiting case of strong repulsion, the single-boson function $G(R) \propto R^{-1/2}$, and the oscillating part of the density correlation function $\tilde{\Pi}(R) \propto R^{-2}$.

As is shown in [15], in the case of weak repulsion the speed of sound can be expressed in terms of the coupling constant c according to Bogolyubov's formula

$$v_s^2 = 2c\rho_B/m_B, \tag{33}$$

where ρ_B and m_B denote the density and mass of the bosons. Expressing the compressibility K in terms of the speed of sound v_S, we find the following result for the exponent α in formulas (27) and (32):

$$\alpha = \frac{1}{2\pi}\left(\frac{2cm_B}{\rho_B}\right)^{1/2}. \tag{34}$$

Thus, the single-boson correlation function falls off slowly in the presence of weak repulsion. The function $\tilde{\Pi}(R)$, corresponding to crystallization, decreases rapidly.

5. COMPARISON WITH OTHER MODELS

In addition to the models with strong interaction considered above, the correlation functions have also been found in a model having a large number of bands[1] and in models having a linear spectrum.[3,4] In the model with a large number of bands, the utilization of the Hamiltonian (21) was justified with the aid of an approximate evaluation of the path integral. For weak attraction, the exponent α in formulas (27) and (32) is given by $\alpha = 1/n$, where n denotes the number of bands. (In [1] the value of the exponent α differs from the correct value by a factor of two, due to an arithmetic error.)

Luther and Emery[4] considered a model with a linear spectrum for the electrons and showed that the Hamiltonian of this model divides in two. One part describes the spin excitations, which are unimportant at low temperatures, since in the case of attraction they have a gap associated with at least one value of the exchange interaction coupling constant. The second part of the Hamiltonian describes the density oscillations and is given by

$$H_0 = 2\pi v_F L^{-1}\sum_k [\rho_1(k)\rho_1(-k)+\rho_2(-k)\rho_2(k)]$$
$$+L^{-1}\sum_k (2V-U_{\|})[\rho_1(k)+\rho_2(k)][\rho_1(-k)+\rho_2(-k)], \tag{35}$$

where ρ_1 and ρ_2 denote the densities of particles with velocity $+v_F$ or $-v_F$. We note that, just as in the Tomonaga model, the last term in expression (35) takes into account besides the term $\sim\rho_1\rho_2$ also the interaction of electrons having equal velocities $\rho_1^2 + \rho_2^2$. The Hamiltonian (35) differs from the Luttinger Hamiltonian, used in [4], by this fact. The Hamiltonian (35) appears more natural to us, since it gives the correct expression for the compressibility $K^{-1} = \pi v + 2V - U_{\|}$ and gives the correct relationship between the speed of sound and the compressibility. After making the change of variables $\rho_1 + \rho_2 = \rho$ and $\pi(\rho_1 - \rho_2) = \bar{\rho}(\nabla\varphi)$, expression (35) goes over into the Hamiltonian (21) of the acoustic excitations. The interaction $2V - U_{\|}$ can evidently be regarded as the Fermi-liquid amplitude, which is related in a complicated manner to the interaction constants of the real Hamiltonian. As is seen from formula (27a), the limiting case of infinitely strong attraction corresponds to the amplitude $2V - U_{\|} = -3\pi v_F/4$. In the low-temperature regime the exponents of the correlation functions, calculated in [4], coincide with those which follow from the hypothesis concerning the role of the acoustic phonons. However, if the gap in the spectrum of the spin excitations is small, a range of temperatures exists, larger than the gap, where the model of Luther and Emery coincides with the Tomonaga model for fermions with spin. In this model the hypothesis concerning the role of acoustic phonons is not valid, since the spin excitations are just as important as the acoustic excitations. Obviously spin excitations are important in all cases when repulsion predominates between the electrons and the spin susceptibility does not tend to zero at low temperatures.

We note that the single-particle Green's functions in the Tomonaga model were calculated in [2], where it was tacitly assumed that the electrons have spin 1/2. Therefore, these functions do not coincide with those which are found in the Tomonaga model for fermions without spin.[3,16]

6. ESTIMATES OF THE SUPERCONDUCTING AND DIELECTRIC TRANSITION TEMPERATURES IN QUASI-ONE-DIMENSIONAL SYSTEMS

In a one-dimensional system there is no long-range order even at zero temperature. However, real systems are quasi-one-dimensional. In such systems an interaction exists between the electrons on different filaments, and there is a tunneling of the electrons from filament to filament. If these effects are relatively

strong, they may lead to a phase transition at high temperatures, where the interaction between the electrons is still small. Below we shall consider the opposite limiting case of a low-temperature transition, when the correlation functions are described by formulas (27) and (32). Here the interaction of the electrons on a single filament is taken into consideration exactly, and the interaction between filaments is taken into account in the self-consistent-field approximation.

The transition into the superconducting state is determined by the tunneling of electrons from one filament to another. Let us denote the amplitude for the hopping of an electron pair from filament i to filament j by W_{ij}. It is proportional to the square of the amplitude for the hopping of an individual electron. Allowing for the hopping events, the Hamiltonian is of the form

$$H=\sum_i H_i+\sum_{i,j} W_{ij}\int b_i^+(x)\,b_j(x)\,dx, \tag{36}$$

where H_i denotes the exact Hamiltonian of a single filament.

In the self-consistent-field approximation, the operators b_i are replaced by the average value $\bar{b}$ of the order parameter for all of the filaments except one. The condition for self-consistency has the form

$$\bar{b}=\frac{\mathrm{Sp}\, b e^{-\tilde{H}/T}}{\mathrm{Sp}\, e^{-\tilde{H}/T}},\quad \tilde{H}=H_i+W\bar{b}\int(b^+ + b)\,dx,\quad W=\sum_j W_{ij}. \tag{37}$$

The transition temperature is determined from the condition for the appearance of a nonvanishing solution of Eq. (37). Expanding the right hand side in a series in powers of $\bar{b}$, we obtain the following equation for the transition temperature

$$1=W\int G(R,\tau)\,dR\,d\tau, \tag{38}$$

where $G(R, \tau)$ is determined by formulas (27) and (27a).

Equation (38) can also be obtained from the condition for instability of the normal state. In the ladder approximation, the equation for the exact, single-boson Green's function $\tilde{G}$ is of the form

$$\tilde{G}(q,\omega)=G(q_\parallel,\omega)\,[1+W(q_\perp)\tilde{G}(q,\omega)]. \tag{39}$$

The limit of instability is found from the condition that the pole of $\tilde{G}$ passes through the point $\omega = 0$. This condition coincides with Eq. (38). Substituting expression (27) into Eq. (38), we obtain the following relationship between the superconducting transition temperature T_c and the amplitude of hopping events:

$$T_c^{2-\alpha}\sim W p_F^{-\alpha}. \tag{40}$$

For strong attraction $\alpha = 1/2$, and for weak attraction $\alpha = 1$; in the last case ϵ_F should be replaced by the transition temperature in the BCS approximation.

In order to estimate the dielectric transition temperature, it is necessary to take into consideration the interaction V_{ij} between electrons on different filaments, which includes both the Coulomb interaction and the interaction via the exchange of phonons. Just as above, in the ladder approximation we obtain the following equation for the density correlation function P:

$$P(q,\omega)=\Pi(q_\parallel,\omega)\,[1+V(q,\omega)P(q,\omega)], \tag{41}$$

where $\Pi(q_\parallel, \omega)$ is determined by formulas (20) and (32). The imaginary part of P is proportional to the cross section for the scattering of neutrons and x rays. The poles of P determine the phonon spectrum, $1 = V(q)\Pi(q_\parallel, \omega)$. The experiment described in [17] indicates that for $q_\parallel \sim 2p_F$ the phonon spectrum weakly depends on $q_\perp$, which confirms the conjecture made above concerning the relative smallness of V(q). At high temperatures the imaginary part of P coincides with the imaginary part of Π and doesn't depend on $q_\perp$. Upon a reduction of the temperature the frequency of the excitations decreases, and for $\omega \ll T$ and $q_\parallel = 2p_F$ we obtain $1 = V(q_\perp)[\Pi(0) + \omega^2 \partial\Pi/\partial\omega^2]$. In this case the frequency strongly depends on $q_\perp$, which also agrees with experiment[17].

In the limit of strong attraction between the electrons on a single filament, $\Pi(q_\parallel, \omega)$ has a strong logarithmic singularity (20). In the intermediate case the singularity is stronger and is determined by formula (32), so that the phonon spectrum has the form $\omega^2 \sim T^2 \times (1 - CT^{2-1/\alpha}/V(q_\perp))$. The temperature at which the phonon spectrum becomes unstable is also the temperature of the dielectric transition. With the aid of the phonon spectrum, let us express the dielectric transition temperature in terms of the interaction potential of the electrons:

$$T_c\sim[\max_\perp V(q_\perp)]^{\alpha/(2\alpha-1)}. \tag{42}$$

If attraction predominates between the electrons on neighboring filaments, then $q_\perp = 0$ for the critical phonons, but if repulsion dominates, a doubling of the lattice period also takes place in the transverse direction.[17] (In analogy with antiferromagnetic and antiferroelectric transitions, such a transition should be called an anti-Peierls transition.)

CONCLUSION

Quasi-one-dimensional systems with a rather strong attraction between the electrons were investigated above. Perhaps potassium-platinum complexes (KCP) constitute such systems. Platinum has a valence of two or four. This may indicate that in compounds of "mixed valence," it is more probable to observe an even number of electrons on each platinum atom. One can assume that such an attraction between the electrons is induced by the exchange of intramolecular vibrations or excitons. The pairs of electrons can be regarded as both superconducting and dielectric fluctuations. It is essential that these fluctuations are quantized. If three-dimensional effects are small, a broad range of temperatures should exist in which the pairs form a liquid. (In KCP this range is found from 100 to 400°.) There is no long-range order in this liquid, but short-range order does exist. At low temperatures the correlation length increases in inverse proportion to the temperature, but the paramagnetic susceptibility should decrease exponentially. In the limit of strong attraction, the conductivity of the electron pairs should be the same as for an ideal gas of spinless fermions, and may have a complicated temperature dependence due to localization of the excitations in one-dimensional systems. If the energy of attraction is of the order of or smaller than the Fermi energy, an additional temperature dependence appears in the cross section for the scattering of an excitation by an individual impurity. The scattering time is proportional to $T^{2-1/\alpha}$. In TTF-TCNQ the interaction between the electrons on a single filament is evidently of the same order as the interaction of the electrons on different filaments. Therefore, the phase transition occurs at those same temperatures, which also correspond to the pairing of the electrons on a single filament. It is difficult to explain the large

maximum in the conductivity by simple ideas about fluctuations, since fluctuation pairs carry currents of approximately the same order as the individual electrons. (Without making artificial assumptions about the long-range nature of the attractive forces or the large number of bands, it is difficult to believe that the value of the index α would be small in comparison with unity.) It is clear that, in order to explain the temperature behavior of the conductivity, it is necessary to have a theory of the localization of strongly interacting electrons.

The experimental data published in [18] indicates that in KCP the specific heat is a linear function of the temperature for $T > 0.15°$. Evidently this means that, due to disorder in the distribution of the Br ions the dielectric transition does not occur and the one-dimensional Bose pairs give a linear contribution to the specific heat. One can explain the small contribution of these pairs to the conductivity by the effects of localization.

Thus, one can surmise that the attraction between the electrons is rather large in KCP and TTF-TCNQ and, for the initiation of superconductivity it is necessary to reduce the dielectric transition temperature and increase the probability for electron hopping from filament to filament. Perhaps one or the other can be achieved by the addition of impurities.

APPENDIX

We shall use the method described in Wu's article[19] in order to prove formula (14). Let us write the determinant in expression (8) in the form

$$[G(R)]^{-1}=\prod_{N=1}^{R-1}x_0^{(N)}, \tag{A.1}$$

where $x_0^{(N)}$ is the solution of the system of equations

$$\sum_{m=0}^{N}g_{n-m-1}x_m^{(N)}=\delta_{0n}, \quad 0\leqslant n\leqslant N. \tag{A.2}$$

Let us apply the Wiener-Hopf method in order to solve Eq. (17). Repeating the calculations carried out in [19], we obtain the following expression for $x_0^{(N)}$:

$$x_0^{(N)}=P(0)Q(0)+\frac{1}{2\pi i}\oint\frac{U(z)Q(z^{-1})z^N}{z}dz. \tag{A.3}$$

Here U(z) is determined by the equation

$$U(\xi)=-\frac{1}{2\pi iP(\xi)}\oint\frac{P(z^{-1})z^N\,dz}{[z-\xi^{-1}(1+\delta)]Q(z)}\left[1-\frac{1}{2\pi i}\oint\frac{Q(z_1^{-1})z_1^NU(z_1)dz_1}{z_1-z^{-1}(1+\delta)}\right]. \tag{A.4}$$

In Eqs. (A.3) and (A.4) the integration is carried out around the unit circle, and δ is a positive infinitesimal quantity. The functions P(z) and Q(z) are analytic inside the unit circle, such that

$$P^{-1}(z)Q^{-1}(z^{-1})=z\,\mathrm{th}\frac{z+z^{-1}-2m\mu}{4mT}. \tag{A.5}$$

For large values of N, Eq. (A.4) can be solved by iterations. However, we shall apply this method only for $NmT \gg \sin p_0$. At low temperatures the singularities of the functions P and Q approach the circumference of the unit circle, and the method of iterations does not work. In formula (A.3) the singularities of the function Q which are close to the circumference of the unit circle are also important; these singularities are found close to the points z_0 and z_0^{-1}, determined from the equation $z_0 + z_0^{-1} = 2m\mu$. For large values of N and any arbitrary relationship between N and T^{-1}, values of z close to z_0 or z_0^{-1} are essential in formula (A.3). These regions can be investigated separately in Eq. (A.4). Thus, in order to determine $x_0^{(N)}$ for $N \gg 1$ it is sufficient to know the function U(z) near the points z_0 and z_0^{-1}. The functions P(z) and $Q(z^{-1})$ have the following form in the neighborhood of these points

$$P(z)=B\left(\frac{1}{2},-\frac{z-z_i}{z_i\beta}\right)\frac{(-1)^i}{\pi z_i}, \qquad Q(z^{-1})=B\left(\frac{1}{2},\frac{z-z_i}{z_i\beta}\right)\frac{z-z_i}{z_i\beta} \tag{A.6}$$

where i = 1, 2, $z_1 = z_0$, $z_2 = z_0^{-1}$, and B(x, y) is the Euler beta function. The parameter β in formulas (A.6) is given by $\beta = 2\pi Tm/\sin p_0$. Substituting the functions P(z) and Q(z) from Eqs. (A.6) in Eqs. (A.3) and (A.4), we obtain a more convenient expression for $x_0^{(N)}$:

$$x_0^{(N)}=e^{\beta/4}\left(1+\frac{2\beta}{\pi^2}\sum_{n=1}^{\infty}\bar{U}_n(N\beta)\right). \tag{A.7}$$

In this expression the new, unknown function of integers, $\bar{U}_n(N\beta)$, is determined by the following system of algebraic equations:

$$\bar{U}_n(N\beta)=e^{-N\beta n}\frac{\Gamma^2(n+1/2)}{\Gamma^2(n)}\sum_{k=0}^{\infty}\frac{e^{-N\beta k}\Gamma^2(k+1/2)}{\Gamma^2(k+1)\,(n+k)}\left[1-\sum_{k_1=1}^{\infty}\frac{\bar{U}_{k_1}(N\beta)}{\pi^2(k_1+k)}\right] \tag{A.8}$$

and is connected by a definite relation with the values of the function U(z) from (A.4) near the points z_0 and z_0^{-1}. We shall not need this relationship in what follows, and therefore we do not present it here.

Comparison of formulas (A.7) and (A.8) enables us to conclude that, for small β and large N but arbitrary βN, the dependence of x_0 on β and N has the form

$$x_0^{(N)}=1+\beta F(\beta N). \tag{A.9}$$

As is clear from formulas (A.1) and (A.2), $x_0^{(N)}$ does not depend on the temperature at low temperatures, $\beta N \ll 1$. Consequently, for small values of βN we find:

$$F(\beta N)=\alpha(\beta N)^{-1}, \quad \beta N\to 0. \tag{A.10}$$

Substituting expressions (A.9) and (A.10) into formula (A.1), we obtain expression (14) for G(R). For large values of βN, one can solve the system of equations (A.8) by iterations. The first four terms of the expansion for the function $F(\beta N)$ are given by

$$F(\beta N)=1/2\,(1/2+e^{-\beta N}+e^{-2\beta N}+e^{-3\beta N}+\ldots). \tag{A.11}$$

We were not able to solve the system (A.8) exactly, but comparison with the hypothesis concerning the role of the acoustic excitations enables us to verify that the coefficients associated with all of the subsequent terms in the expansion (A.11) are equal to unity. Therefore, $F(\beta N) = (1/4)\coth(\beta N/2)$, and we obtain expression (28) for G(R). In any case comparison with Szegö's formula shows that the coefficient α in formula (A.10) is equal to 1/2. For bands which are half filled, the correlation function (A.10) coincides with the correlation function of the XY-model.

It is asserted in [20] that at zero temperature the correlation function of this model falls off exponentially with distance. Such a result is a consequence of a calculational error. The correct calculation of expression (24) in this article leads to a power-law decrease.

[1] K. B. Efetov and A. I. Larkin, Zh. Eksp. Teor. Fiz. **66**, 2290 (1974) [Sov. Phys.-JETP **39**, 1129 (1974)].
[2] I. E. Dzyaloshinskiĭ and A. I. Larkin, Zh. Eksp. Teor. Fiz. **65**, 411 (1973) [Sov. Phys.-JETP **38**, 202 (1974)].
[3] A. Luther and I. Peschel, Phys. Rev. **B9**, 2911 (1974).
[4] A. Luther and V. J. Emery, Phys. Rev. Lett. **33**, 589 (1974).

[5]M. Gaudin, Phys. Lett. **24A**, 55 (1967); C. N. Yang, Phys. Rev. Lett. **19**, 1312 (1967); E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[6]M. Girardeau, J. Math. Phys. **1**, 516 (1960).
[7]D. C. Mattis, The Theory of Magnetism, Harper & Row, 1965 (Russ. Transl., "Mir", 1968).
[8]U. Grenander and G. Szegö, Toeplitz Forms and Their Applications, University of California Press, 1958 (Russ. Transl., IIL, M. 1961).
[9]P. A. Lee, T. M. Rice, and P. W. Anderson, Phys. Rev. Lett. **31**, 462 (1973).
[10]V. G. Vaks, A. I. Larkin, and S. A. Pikin, Zh. Eksp. Teor. Fiz. **51**, 361 (1966) [Sov. Phys.-JETP **24**, 240 (1967)].
[11]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. **B6**, 3409 (1972).
[12]R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill Book Company, 1965 (Russ. Transl., Mir, 1968).
[13]H. Shiba, Prog. Theor. Phys. **48**, 2171 (1972).
[14]V. Ya. Krivnov and A. A. Ovchinnikov, Zh. Eksp. Teor. Fiz. **67**, 1568 (1974) [Sov. Phys.-JETP **40**, 781 (1975)].
[15]E. H. Lieb, Phys. Rev. **130**, 1616 (1963).
[16]H. U. Everts and H. Schulz, Solid State Commun. **15**, 1413 (1974).
[17]R. Comes, M. Lambert, and H. R. Zeller, Phys. Status Solidi **58**, 587 (1973).
[18]W. A. Reed, F. S. L. Hsu, R. J. Schutz, J. E. Graebner, and H. J. Guggenheim, Phys. Rev. Lett. **34**, 473 (1975).
[19]T. T. Wu, Phys. Rev. **149**, 380 (1966).
[20]V. M. Kontorovich and V. M. Tsukernik, Zh. Eksp. Teor. Fiz. **52**, 1446 (1967) [Sov. Phys.-JETP **25**, 960 (1967)].

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