Thermodynamics of interacting electrons in disordered one-dimensional conductors

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(Submitted 9 August 1979)
Zh. Eksp. Teor. Fiz. 78, 812–830 (February 1980)

Assuming the electron interaction to be sufficiently weak and short range, we succeed in solving exactly the problem of the temperature behavior of the thermodynamic quantities for quasi-one-dimensional electrons in a system with disorder. Since all the electronic states are localized in the presence of defects, the interaction leads to a number of singularities in the low-temperature properties of the specific heat, susceptibility, and others. Thus, in the case of repulsion, a region where the Curie law holds appears for the magnetic susceptibility. It is shown that in real compounds a major role is played by spatial correlations between the occupation numbers of individual localized states.

PACS numbers: 71.50. + t, 75.30.Cr

1. INTRODUCTION AND FORMULATION OF PROBLEM

Until recently, mathematical difficulties have made it impossible to take exactly into account the interactions between electrons in a one-dimensional system with a disorder due to some static defects (impurities, crystal imperfections, and others). The present paper is the first attempt in this direction by using a method developed by us earlier (henceforth cited as I).

In addition to the general physical interest of the problem itself, we have in mind also the curious properties which were observed experimentally in the low-temperature region in the compounds NMP-, Ad-, and Qn-TCNQ.[2]

As noted in Ref. 3, these substances have degenerate internal disorder because of the nonsymmetry of one of the components—the cation. The nonsymmetry of the cation molecules in these compounds is due to the presence of either one extra nitrogen atom or of the CH_3 group, which can occupy randomly crystal any one of two possible positions. We make immediately the following remark: in these compounds we are dealing with rather large flat molecules, as a result of which the aforementioned asymmetry is in a certain sense small. If in addition the conductivity is due primarily to the motion of the electrons along the TCNQ filaments, as is apparently the case (see, however, Ref. 4), then the additional group is in turn located relatively far from the conducting chain. These are apparently sufficient reasons for assuming the mean free path in them to be large enough.

The peculiarity of the properties of the aforementioned compounds, compared with such typical good conductors as TTF-TCNQ, lies in particular in the fact that no structural (Peierls) transition takes apparently place in them at higher temperatures. The most pronounced phenomenon observed in these compounds can be taken to be the singularities in the behavior of a number of thermodynamic quantities, primarily the susceptibility, which shows in the temperature interval from 5 to 0.2 K a rapid growth reminscent of the Curie law, but with a different exponent: $\chi \propto T^{-\alpha}$, where $\alpha = 0.58$, 0.74, and 0.75 for NMP-, Ad-, and Qn-TCNQ, respectively.

A number of explanations have been proposed for this behavior.[2] One is that the conduction band in these compounds is exactly one-half or one-quarter filled, i.e., the Fermi level of the electrons occupies a special (commensurate) position in the band. An analysis[5] has shown that disorder is in fact capable of leading to a singularity in the single-particle state density, but only for a half-filled band. At a smaller commensurability of the Fermi momentum, the maxima that appear in the state density cannot describe the susceptibility temperature dependences observed in Ad- and Qn-(TCNQ)$_2$. Doubts have been expressed recently concerning the very fact of the fractional occupation of the conduction band in these compounds.[4]

Another explanation, proposed in Refs. 2 and 6, presumes, on the contrary, that the disorder introduced by the cation is large enough compared with the width of the band, as a result of which the electrons are distributed, in first-order approximation, one each on the corresponding TCNQ molecule, and their spins are weakly correlated, in proportion to a correction that is quadratic in the ratio of the exchange integral to the characteristic scatter of the energy levels of the individual wells. The weak spot of this approach is that the conductivity of these compounds is far from small and has a noticable temperature dependence, and indicated anomalies temperature regularities appear only at sufficiently low temperatures.

In the present paper, in accord with the foregoing, we shall assume the disorder to be small enough compared with the width of the conduction band and use only the fact that in a one-dimensional system, in the presence of static defects, all the electronic states are localized.[7,8] We consider here, of course, a simplified model of interactions between localized electrons. Thus, the interaction is assumed to be sufficiently weak. However, the principal simplification of the model lies in the assumption that the interaction potential is short-range, something apparently not always satisfied in a real quasi-one-dimensional crystal. (For a single filament our results could be easily generalized also to include the case of Coulomb interaction.)

0038-5646/80/020409-09$02.40

The physical phenomenon investigated in this paper consists in the fact that the repulsion makes it impossible for two electrons to occupy separate energy states that are sufficiently close to the Fermi level; this leads to the appearance of a small number of unpaired spins. In turn, the attraction inevitably pairs the electrons and leads to a rapid decrease of the susceptibility at low temperatures. We succeeded in carrying through to conclusion the actual calculation of the mean values that appear in the problem, using the method developed in I for averaging the products of exact eigenfunctions of electrons.

The degree to which the results obtained in the article are general are discussed in the concluding section.

2. SELECTION OF PRINCIPAL-APPROXIMATION TERMS

As will be seen later on, by assuming the interaction potential between the electrons to be short-range (atomic scale), it suffices to consider in a quasi-one-dimensional crystal only a single filament. The filaments can be regarded as independent in the sense of the distribution of the defects, and the electronic states can be regarded as localized on only one filament. To simplify the estimates we choose the interaction potential $u(x)$ for the time being in the form $u(x) = u_0 \delta(x)$. The corresponding Hamiltonian of the interaction takes in the second quantization the form

$$\frac{1}{2} u_0 \int \psi_\sigma^+(x)\psi_{-\sigma}^+(x)\psi_{-\sigma}(x)\psi_\sigma(x)\,dx.$$

We examine the character of the corrections to any quantity, say the magnetic susceptibility χ. These corrections are given by the diagram series shown in Fig. 1. The matrices $\hat{\sigma}$ in the vertices are Pauli matrices. To understand the meaning of the indices marked on the lines corresponding to the electron Green's functions, we must recall that in the discrete representation, i.e., for localized states, the electron Green's function takes the form

$$G_{i\omega_n}(x, x') = \sum_\nu \frac{\psi_\nu(x)\psi_\nu(x')}{i\omega_n - \varepsilon_\nu},$$

where the sum is taken over all the eigenstates of the given realization of the random potential.

As usual, each diagram contains, besides the sums over the energy levels $\varepsilon_\nu, \varepsilon_\mu$, etc., also summation over the Matsubara frequencies. The diagrams are written in accordance with the usual diagram-technique rules.[9] According to I, it turns out that in the sums over the energies for the individual diagrams of Fig. 1 a special role is played by terms with equal indices. Thus, if we compare the second diagram of Fig. 1 at $\mu \neq \nu$ with the first diagram of Fig. 2, then we obtain respectively the following two expressions (disregard-
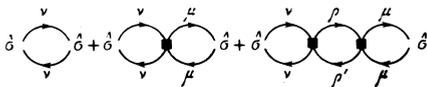
FIG. 1.
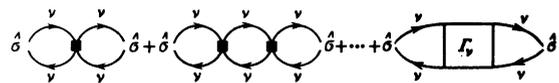
FIG. 2.

ing numerical coefficients):

$$\mu^2 \sum_{\nu,\mu} \frac{u_0}{T^2} \mathrm{ch}^{-2}\frac{\varepsilon_\nu}{2T} \mathrm{ch}^{-2}\frac{\varepsilon_\mu}{2T} \psi_\nu^2(x) \int \psi_\nu^2(y)\psi_\mu^2(y)\,dy\,\psi_\mu^2(x')$$

and

$$\mu^2 \sum_\nu \frac{u_0}{T^2} \mathrm{ch}^{-4}\frac{\varepsilon_\nu}{2T} \psi_\nu^2(x) \int \psi_\nu^4(y)\,dy\,\psi_\nu^2(x').$$

For the correction to the susceptibility (i.e., integrating with respect to x' and averaging) we obtain

$$\mu^2 \nu(E_F)\frac{u_0}{T^2} \int d\varepsilon_\nu \,\mathrm{ch}^{-2}\frac{\varepsilon_\nu}{2T} \sum_\mu \mathrm{ch}^{-2}\frac{\varepsilon_\mu}{2T} \left\langle \int \psi_\nu^2(y)\psi_\mu^2(y)\,dy \right\rangle_U$$

and

$$\mu^2 \nu(E_F)\frac{u_0}{T^2} \int d\varepsilon_\nu \,\mathrm{ch}^{-4}\frac{\varepsilon_\nu}{2T} \left\langle \int \psi_\nu^4(y)\,dy \right\rangle_U.$$

In order of magnitude we have

$$\int \psi_\nu^4(y)\,dy \sim l^{-1};$$

analogously we obtain

$$\int \psi_\nu^2(y)\psi_\mu^2(y)\,dy \sim l^{-1},$$

if the "centers" of the states ν and μ are separated by a distance of the order of l. Therefore the number of significant terms in the sum over μ is estimated as the product of the state density $\nu(E_F)$ by the energy interval $\sim T$ [because of $\cosh^{-2}(\varepsilon/2T)$] and by the volume l, i.e.,

$$\Delta N \sim \nu(E_F) T l.$$

Thus, the contribution of the first term ($\mu \neq \nu$) is $\sim \nu^2(E_F)u_0 = \nu(E_F)g$ (where $u_0/\pi v = g$ is a dimensionless constant) and has the usual meaning of the renormalization of the susceptibility, just as for free electrons,[1] whereas the contribution of the first diagram of Fig. 2 is

$$\mu^2 \nu(E_F)g/\tau T$$

and predominates generally speaking at low temperatures. This term becomes large at

$$g/\tau T \sim 1. \tag{1}$$

The renormalization constants are not of great interest to us. At the same time, it is easy to verify (see below) that *any* diagram of Fig. 2 with identical indices yields terms of the form $(g/\tau T)^n$. Thus, the temperature behavior of the susceptibility and of other quantities at sufficiently low temperature calls for summation of a series of diagrams of Fig. 2 over the powers of the parameter (1).

We shall check also on some diagrams of the "mixed" type, for example those shown in Fig. 3. As to the second of them, its contribution, as follows from the preceding, is of the order of the contribution of the first diagram of Fig. 2, multiplied by g (i.e., $g^2/\tau T$). For the first diagram of Fig. 3 we obtain the expression
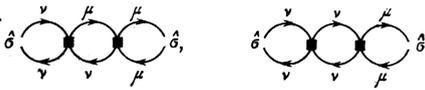
FIG. 3.

$$\sum_{\mu,\nu}\frac{u_0{}^2}{T^2}\,\mathrm{ch}^{-2}\frac{\varepsilon_\nu}{2T}\,\mathrm{ch}^{-2}\frac{\varepsilon_\mu}{2T}\frac{\mathrm{th}\,(\varepsilon_\mu/2T)-\mathrm{th}\,(\varepsilon_\nu/2T)}{\varepsilon_\mu-\varepsilon_\nu}$$

$$\times\psi_\nu{}^2(x)\int\psi_\nu{}^3(y)\,\psi_\mu(y)\,dy\int\psi_\mu{}^3(z)\,\psi_\nu(z)\,dz\psi_\mu{}^2(x').$$

Estimating the sum as above, we again find that its relative contribution to the susceptibility is $g^2/\tau T$.

Thus, if the summation of the principal terms yields a function of the type $f(g/\tau T)$, then the considered mixed-type diagrams will be gathered into functions of the form $gf_1(g/\tau T)$.

All the estimates made above with individual diagrams as the example can be easily formulated for an arbitrary term of the series. The result of summation over the frequencies leads to the usual formulas of quantum-mechanical perturbation theory. Therefore, if we have the diagram with p interactions and m independent energy indices, then the matrix element of the interaction introduces a factor $(g/\tau)^p$, and the energy denominators introduce a factor T^{-p} into the estimate of the individual term in the sum. Finally, the number of significant terms in m summations is

$$(\nu(E_F)Tl)^m\sim(T\tau)^m.$$

Thus, the expansion in powers of g actually extends over the number of independent energy indices:

$$g^{m-1}f_{m-1}(g/\tau T).$$

We have no expressions for the functions $f_m(g/\tau T)$, and therefore, strictly speaking, the temperature region for which the results that follow are valid is determined by the conditions

$$g/\tau T\gtrsim 1,\qquad g^2/\tau T\ll 1. \tag{2}$$

Nonetheless, qualitative arguments can be advanced favoring the assumption that the results obtained below are valid in a temperature region larger than (2). The fact that in all the diagrams the main contribution is due to terms with the same state index ν means that we are dealing simply with the energy of interaction between two electrons having opposite spins on one and the same energy level. This energy is small ($\sim g/\tau$) not only compared with the Fermi energy, but also, by virtue of the weakness of the interaction $g\ll 1$, with the average distance $\sim 1/\tau$ between neighboring levels. Therefore at the temperatures defined by relation (1) most levels are either already occupied by two electrons or empty, with the exception of those rare states whose energies turn out to be in the interval $\sim g/\tau$ near the Fermi level. The number of such states (per unit length) is $\nu(E_F)|g|\tau$, and consequently the average distance between these levels is

$$\bar R\sim l/g. \tag{3}$$

Recognizing that the wave functions decrease exponentially at large distances, the matrix elements of functions of such states are exponentially small and we

might expect the temperatures at which the correlation between such states becomes significant are exponentially small like $\exp(-|g|^{-1})$. If this argument is correct, then the terms of the type $gf_1(g/\tau T)$ are small of order g not only for (2) but in the entire indicated temperature interval.

So far we have said nothing concerning the corrections to the electron Green's functions, for example those shown in Fig. 4. For electrons without impurities, the principal terms in this diagram, just as in higher-order diagrams, reduce to an average shift of the chemical potential ($\Delta\mu\sim gE_F$). In the presence of defects, the chemical potential, of course, fluctuates in the vicinity of each localized state. The order of magnitude of this fluctuation is g/τ, i.e., a quantity of the same order as the temperature scale of interest to us. It is easily understood, however, that these fluctuations are insignificant, since their magnitude does not depend on the temperature. They comprise merely some additional static random field. In fact, we have explained above that each level arbitrarily close to the chemical potential, as required by condition (1), is surrounded by levels whose occupation does not depend on temperature, including those independent of the degree of occupation of the first level, since the fluctuation energy g/τ is less than the average distance $1/\tau$ between them.

It must finally be noted that when we single out terms of the type $(g/\tau T)^n$ we imply that they constitute the principal singularity. Yet it is well known[10] that, in the absence of defects, a system of interacting electrons is characterized by logarithmic divergences. The corresponding corrections are of the order of $g\ln(E_F/T)$ and are due to effects of Cooper and dielectric pairing. Similar divergences exist at least in the Cooper channel also in the presence of defects (they are due to the Cooper diagrams with noncoincident indices). This in turn imposes limitations either on the temperature (at low impurity concentration)

$$g\ln(E_F/T)\ll 1, \tag{4}$$

or on the impurity concentration, when it comes to temperatures defined by condition (1) or (3):

$$g\ln(E_F\tau)\ll 1. \tag{4'}$$

These conditions will hereafter be assumed satisfied.

3. ELECTRON INTERACTION ON LOCALIZED STATES

The preceding discussion is sufficient for a final formulation of the problem. The needed term in the diagram series can be described with the aid of the following interaction Hamiltonian:

$$H_{int}=\sum_\nu A_\nu\hat a_{\nu\uparrow}{}^+\hat a_{\nu\downarrow}{}^+\hat a_{\nu\downarrow}\hat a_{\nu\uparrow}, \tag{5}$$

where A_ν denotes the matrix element

$$A_\nu=\iint dxdx'\psi_\nu{}^2(x)u(x-x')\psi_\nu{}^2(x'). \tag{6}$$

FIG. 4.

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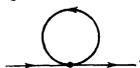
The contribution of the level ν to the thermodynamic potential is

$$\Omega_\nu = -T \ln Z_\nu,$$

where

$$Z_\nu = \mathrm{Sp} \exp\left\{ -\frac{1}{T}\left[\sum_\sigma \varepsilon_{\nu\sigma}\hat{a}_{\nu\sigma}^+\hat{a}_{\nu\sigma} - A_\nu \hat{a}_{\nu\uparrow}^+\hat{a}_{\nu\uparrow}\hat{a}_{\nu\downarrow}^+\hat{a}_{\nu\downarrow} \right]\right\}. \tag{7}$$

The trace in (7) must be taken over the following set of occupation numbers:

$$(n_\uparrow, n_\downarrow) = (0,0;\ 1,0;\ 0,1;\ 1,1).$$

We have included in the level energy, to generalize the results, also the term due to the interaction with the magnetic field:

$$\varepsilon_{\nu\sigma} = \varepsilon_\nu + \mu(H\hat{\sigma}).$$

This yields directly

$$Z_\nu = 1 + 2\exp\left(-\frac{\varepsilon_\nu}{T}\right)\mathrm{ch}\frac{\mu H}{T} + \exp\left(-\frac{2\varepsilon_\nu + A_\nu}{T}\right).$$

The thermodynamic potential of the entire system is

$$\Omega = -T\int d\xi \left\langle \ln\left[1 + 2\exp\left(-\frac{\xi}{T}\right)\mathrm{ch}\frac{\mu H}{T} + \exp\left(-\frac{2\xi + A(\xi)}{T}\right)\right]\right.$$
$$\left. \times \sum_\nu \delta(\xi - \varepsilon_\nu)\right\rangle_U \tag{8}$$

where the symbol $\langle \ldots \rangle_U$ corresponds to averaging over all the realizations of the random potential.

In the quasiclassical energy region $k_F l \gg 1$ the distribution of the probabilities of the quantity A_ν (6) does not depend on energy. We rewrite expression (8) therefore in the form

$$\Omega \equiv (2L)\tilde{\Omega} = -(2L)T\nu(E_F)\int d\xi \int dA\, w(A)$$
$$\times \ln\left[1 + 2\exp\left(-\frac{\xi}{T}\right)\mathrm{ch}\frac{\mu H}{T} + \exp\left(-\frac{2\xi + A}{T}\right)\right], \tag{8'}$$

where $2L$ is the length of the chain. We have thus introduced the probability distribution function for the quantity A_ν of (6):

$$w(A) = (\nu(E_F)2L)^{-1}\left\langle \sum_\nu \delta(A - A_\nu)\delta(\xi - \varepsilon_\nu)\right\rangle_U. \tag{9}$$

The presence of the energy δ-function in (8) and (9) reflects the fact that ε_ν is an eigenvalue of the energy at the given realization of the random potential.

The determination of the last mean value, i.e., of the function $w(A)$ of (9), is in fact the subject of the paper. Before we proceed to do so, however, we obtain in this section, using the representation (8), expressions for the basic thermodynamic quantities.

The simplest expression is obtained for the magnetic moment in an external magnetic field:

$$M = -(\partial\tilde{\Omega}/\partial H)_T = 2\mu\,\mathrm{sh}(\mu H/T)\nu(E_F)$$
$$\times \int d\xi \left\langle \frac{\exp(-\xi/T)}{1 + 2\exp(-\xi/T)\mathrm{ch}(\mu H/T) + \exp[-(2\xi + A)/T]}\right\rangle.$$

[The averaging symbol in this and all the following expressions will henceforth denote, according to (8'), averaging with the function $w(A)$.] The integral with respect to ξ in the last expression can be evaluated ex-

plicitly; the result, however, depends on the assumption concerning the sign of the interaction.

Repulsion between electrons ($A > 0$)

We have

$$M = \mu\nu(E_F)T\,\mathrm{sh}\frac{\mu H}{T}\left\langle \frac{\exp(A/T)}{R(A)}\ln\left[\frac{\mathrm{ch}(\mu H/T)\exp(A/T) + R(A)}{\mathrm{ch}(\mu H/T)\exp(A/T) - R(A)}\right]\right\rangle,$$
$$\tag{10}$$
$$R(A) = [\exp(A/T)(\mathrm{ch}^2(\mu H/T)\exp(A/T) - 1)]^{1/2}.$$

At the lowest temperatures[2]

$$M = \mu\nu(E_F)T\,\mathrm{th}(\mu H/T)[\ln(4\,\mathrm{ch}^2(\mu H/T)) + \langle A\rangle/T]. \tag{10'}$$

From (10) we get for the susceptibility χ in weak fields

$$\chi = \mu^2\nu(E_F)[\langle A\rangle T^{-1} + 2\ln 2]. \tag{10''}$$

At $H \neq 0$ and $T \to 0$ we obtain for the magnetization

$$M = \mu\nu(E_F)[2\mu H + \langle A\rangle + T2\ln 2]. \tag{11}$$

The term linear in the field corresponds to the Pauli susceptibility whereas the constant term describes the contribution of the independent localized spins that become polarized in the absence of interaction between them at $T = 0$ even in an arbitrarily weak field. We have already advanced arguments that these interactions become significant only at exponentially low temperatures. Corresponding lower bounds appear in (11) also on the field intensity.

Attraction between electrons ($A < 0$)

In place of (10) we obtain

$$M = 2\mu\nu(E_F)T\,\mathrm{sh}\left(\frac{\mu H}{T}\right)\left\langle \left[\exp\left(\frac{A}{T}\right)\left(1 - \mathrm{ch}^2\left(\frac{\mu H}{T}\right)\exp\left(\frac{A}{T}\right)\right)\right]^{-1/2}\right.$$
$$\left. \times \left[\frac{\pi}{2} - \mathrm{arc\,tg}\left(\frac{\exp(A/T)}{[\exp(A/T)(1 - \mathrm{ch}^2(\mu H/T)\exp(A/T))]^{1/2}}\right)\right]\right\rangle.$$

The susceptibility is $\tag{12}$

$$\chi = 2\mu^2\nu(E_F)\left\langle \left[\exp\left(\frac{A}{T}\right)\left(1 - \exp\left(\frac{A}{T}\right)\right)\right]^{-1/2}\right.$$
$$\left. \times \left[\frac{\pi}{2} - \mathrm{arc\,tg}\left(\frac{\exp(A/T)}{[\exp(A/T)(1 - \exp(A/T))]^{1/2}}\right)\right]\right\rangle$$

and behaves at the very lowest temperatures like

$$\chi \approx \pi\mu^2\nu(E_F)\langle\exp(A/2T)\rangle. \tag{13}$$

We call attention to the fact that the radicand in (12) can reverse sign, depending on the ratio of the electron interaction energy A and the field μH [in this case it is necessary to change over again from (12) to (10)]. The physical interpretation of this phenomenon is obvious: a sufficiently strong field is capable of overcoming the electron interaction energy in the localized state and break a pair of compensated spins.

At a fixed field μH and at $T = 0$ all the pairs whose interaction energy is subject to the inequality $2\mu H > |A|$ are broken. Going again to the limit $T = 0$ in (10) we obtain

$$M(H) = \mu\nu(E_F)\int_0^{|A| = 2\mu H} (2\mu H + A)w(A)\,dA. \tag{14}$$

We proceed now to the equations for the specific heat. Since we are dealing with low temperatures we need not distinguish, by virtue of the Nernst theorem, between the specific heats at constant volume, say, or constant

pressure, and we can calculate directly[3]

$$c=-T(\partial^2\Omega/\partial T^2)_\mu.$$

Differentiation of (8) with respect to temperature makes it possible, after a number of straight forward but somewhat cumbersome calculations, to transform the expression for the specific heat to the following fairly symmetrical integral:

$$c=4\nu(E_F)T\left\langle \exp\left(\frac{A}{2T}\right)\int_0^1\frac{dv}{[v^2+2v\exp(A/2T)+1]^2}\right.$$
$$\left.\times\left\{v^3\left(\ln v-\frac{A}{2T}\right)^2+2v\ln^2 v\exp\left(-\frac{A}{2T}\right)+\left(\ln v+\frac{A}{2T}\right)^2\right\}\right\rangle, \quad (15)$$

which in principle can be calculated in closed form. Since the remaining expression is still quite complicated, we consider again the limiting case of low temperatures. We recall that $A\equiv 0$, i.e., for the specific heat of noninteracting electrons, we have a linear temperature law:

$$c={}^2/_3\nu(E_F)\pi^2T, \quad A=0. \quad (16)$$

In the case of repulsion $\exp(-A/T)\to 0$ and the main contribution is due to the third term in the integrand of (15), with the principal role assumed by small v. This preserves the linear dependence of the specific heat on the temperature, but the coefficient is changed:

$$c={}^2/_3\nu(E_F)\pi^2(1+6\pi^{-2}\ln^2 2)T, \quad A>0. \quad (16')$$

Finally, for an attraction interaction, $\exp(-A/T)\to\infty$ and the principal role in (15) is played by $v\sim 1$. The main contribution is made by the first term in the integrand of (15). We again obtain the linear law

$$c=\nu(E_F)(\pi^2/6)T, \quad A<0. \quad (16'')$$

To understand the nature of the resultant state, interest attaches also to the function that expresses the law of occupation $n(\xi)$ of the states with energy ξ:

$$n(\xi)=2\frac{\exp(-\xi/T)+\exp[-(2\xi+A)T]}{1+2\exp(-\xi/T)+\exp[-(2\xi+A)/T]}. \quad (17)$$

We consider only the case of absolute zero temperature. We then have for repulsion

$$n(\xi)=\begin{cases} 2, & \xi<-A \\ 1, & -A<\xi<-A/2. \\ 0, & \xi>-A/2 \end{cases} \quad (17')$$

For attraction

$$n(\xi)=\begin{cases} 2, & \xi<-A/2 \\ 0, & -A/2<\xi \end{cases}. \quad (17'')$$

The calculation of the mean value $\langle n(\xi)\rangle$ calls for knowledge of the function $w(A)$. At any rate, it is seen from (17') and (17'') that the Fermi step becomes smeared out. This smearing covers, however, a small vicinity of the Fermi surface. The particle-number density N (for a given chemical potential)

$$N=\nu(E_F)\int_{-\infty}^\infty\langle n(\xi)\rangle d\xi,$$

changes insignificantly. The corresponding changes of the chemical potential (in terms of the variables N and T) are therefore also small, so that all the thermodynamic quantities can be calculated at a constant chemical potential.

4. CALCULATION OF THE MEAN VALUES

Before we proceed directly to the calculations, we simplify expression (6) for the quantity A, assuming as before a short-range interaction potential $u(x)$. Following the article I, we write down the eigenfunctions $\psi_\nu(x)$ in the form[4]

$$\psi_\nu(x)=R(x)\sin\varphi(x).$$

The phase $\varphi(x)$ of the wave function contains a rapidly oscillating part $\varphi_0(x)=k_Fx$, which must be averaged in the integral (6). As a result we obtain

$$A_\nu=g_{eff}\left(\frac{\pi v}{4}\right)\int R_\nu^4(x)dx, \quad g_{eff}=g_2+\frac{g_1}{2}, \quad (6')$$

where we have introduced the dimensionless constants $g_1=(\pi v)^{-1}u_{2k_F}$ and $g_2=(\pi v)^{-1}u_0$, so as to establish a correspondence with the notation of Ref. 10. It was noted in Ref. 10, in particular, that the interaction can always be divided into two parts corresponding, for free electrons, to scattering of the electrons by one another either with small momentum transfer (g_2), or of the order of $\pm 2k_F$ (g_1). Thus, according to (6'), the sign of the effective interaction is determined by the sum of both constants.

We write the probability distribution $w(A)$ (9) in the form

$$w(A)=\frac{1}{2\pi i}\int_C e^{\lambda A}w_\lambda d\lambda. \quad (18)$$

Here C is the Laplace contour $(-i\infty+\delta,+i\infty+\delta)$. If $g_{eff}>0$ (repulsion), the Laplace transform

$$w_\lambda=(\nu(E_F)2L)^{-1}\left\langle\sum_\nu\exp(-A_\nu\lambda)\delta(\xi-\varepsilon_\nu)\right\rangle_U \quad (19)$$

is defined as an analytic function in the right-hand half-plane of a complex variable λ ($\mathrm{Re}\,\lambda>0$). In C we have correspondingly $\delta>0$. In the opposite case of attraction $(g_{eff}<0)$, w_λ is analytic in the left-hand half-plane of λ, $\mathrm{Re}\,\lambda<0$, and the integration in the inverse of the Laplace transform (18) is along the imaginary axis, but $\delta<0$.

We now expand the exponential of (19) formally in a series. We consider an arbitrary term of n-th order:

$$\frac{(-\lambda)^n}{\nu(E_F)2Ln!}\left\langle\sum_\nu A_\nu^n\delta(\xi-\varepsilon_\nu)\right\rangle_U$$
$$=\frac{(-\lambda g_{eff}\pi v)^n}{2L\nu(E_F)\cdot 4^n}\left\langle\int_{-L}^L dx_nR^4(x_n)\ldots\int_{x_3}^L dx_2R^4(x_2)\right.$$
$$\left.\times\int_{x_2}^L dx_1R^4(x_1)v^{-1}[\delta(\varphi^>-\varphi^<)(\zeta^>-\zeta^<)]_x\right\rangle_U. \quad (20)$$

In (20) we have transformed the sum over the energy eigenvalues in accord with (27) of I. The fact that the wave function is an eigenfunction is expressed now by the condition that the phases of the wave function $\varphi^>(x)$ and $\varphi^<(x)$, obtained by solving the Schrödinger equation from the left and from the right, coincide at an arbitrarily chosen junction point x_0 accurate to an integer multiple of π.

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The factorial multiplier has also dropped out of (20) because all the coordinates are arranged in increasing order in the integrals ($x_n < x_{n-1} < \ldots < x_3 < x_2 < x_1$).

From among the equations of article I we shall need [(19), I]

$$R(x_i) = \alpha(x_i|x_0)R(x_0),$$

where $R(x_0)$ is a normalization factor [(26), I]:

$$R^2(x_0) = 2[\zeta^> - \zeta^<]_{x_0}^{-1}.$$

(All the eigenfunctions are normalized to unity.)

Obviously, it is convenient to choose in (20) the junction point at $x_1 (x_0 \equiv x_1)$. The mean value (20) depends only on the difference between the coordinates at $2L \to \infty$. After averaging, one of the integrations cancels out the total chain length $2L$ from the denominator of (20). Using all this and the fact that $\nu(E_F) = (\pi v)^{-1}$ we obtain for (20)

$$\pi(2L)^{-1}(-\lambda)^n(g_{eff}/\pi v)^n \left\langle \int_{-L}^{L} dx_n \alpha^4(x_n|x_1) \right.$$

$$\ldots \int_{x_3}^{L} dx_2 \alpha^4(x_2|x_1) \int_{x_2}^{L} dx_1 [\delta(\varphi^> - \varphi^<)(\zeta^> - \zeta^<)^{1-2n}]_{x_1} \left. \right\rangle .$$

We rewrite the last expression, using the property

$$\alpha(x_1|x_2) = \alpha(x_1|y)\alpha(y|x_2)$$

and the transformation

$$[\zeta^> - \zeta^<]_{x_1}^{-1} = \int_0^\infty \exp(-s[\zeta^> - \zeta^<]_{x_1}) ds.$$

After making the substitutions we get

$$\frac{\pi}{2L}\frac{(-\lambda g_{eff}/\pi v)^n}{(2n-2)!} \int_0^\infty s^{2n-2} ds \left\langle \int_{-L}^{L} dx_n \alpha^4(x_n|x_1) \right.$$

$$\ldots \int_{x_3}^{L} dx_2 \alpha^{4(n-1)}(x_2|x_1) \int_{x_2}^{L} dx_1 \exp[-s\zeta^>(x_1)]$$

$$\times \delta(\varphi^>(x_1) - \varphi^<(x_1)) \exp[s\zeta^<(x_1)] \left. \right\rangle_v .$$

In turn,

$$\delta(\varphi^>(x_1) - \varphi^<(x_1)) = \int d\varphi \delta(\varphi^>(x_1) - \varphi)\delta(\varphi - \varphi^<(x_1)).$$

The purpose of all the transformations was to represent the general expression (20) in the form of a product of two factors, the averaging of which could be carried out independently by using the Markov character of the random process[5]:

$$\int_{x_2}^{\infty} dx_1 \int_0^\infty ds \int_{-\pi/2}^{\pi/2} \frac{d\varphi}{\pi} K^{(n-1)}(s, \varphi|x_1 - x_2) Q^{(0)}(s, \varphi), \qquad (21)$$

where

$$Q^{(0)}(s, \varphi) = \pi \langle \exp[s\zeta^<(x_1)] \delta(\varphi - \varphi^<(x_1)) \rangle_v,$$

$$K^{(n-1)}(s, \varphi|x_1 - x_2) = \frac{\pi(g_{eff}\pi v)^n s^{2(n-1)}}{(2L)(2n-2)!} \left\langle \int_{-L}^{L} dx_n \alpha^4(x_n|x_1) \right.$$

$$\ldots \int_{x_3}^{L} \alpha^{4(n-1)}(x_2|x_1) dx_2 \exp[-s\zeta^>(x_1)] \delta(\varphi^>(x_1) - \varphi) \left. \right\rangle_v .$$

The boundary condition in the last expression with respect to $R = x_1 - x_2$

$$K^{(n-1)}(s, \varphi|x_1 = x_2) = -\frac{g_{eff}\pi v s^2}{(2n-2)(2n-3)} \int_0^\infty K^{(n-2)}(s, \varphi|R) dR. \qquad (22)$$

The equation for the function $K^{(n-1)}(s, \varphi|R)$ can be written by considering its variations with changing x_1. We shall not present here the rather simple derivation, which is entirely based on Eqs. (36) and (54) of article I (or on the equivalent equations for a Gaussian potential). The final expression turns out to be quite simple:

$$l\frac{\partial K^{(n)}}{\partial R} = 2s^2 \frac{\partial^2 K^{(n)}}{\partial s^2} - (ls) K^{(n)}. \qquad (23)$$

(The definition of l in I is such that $l = 2l_0$, where l_0 is the kinetic mean free path.)

Since the quasiclassical approach is used, $k_F l \gg 1$, the dependence on the phase φ drops out in fact from all the quantities in the case when only one proper energy level is involved. The phase distribution probability $w(\varphi)$ is simply

$$w(\varphi) = \pi^{-1}.$$

Before we continue with the calculations, let us simplify the notation, and take into account in particular also this last fact. We introduce the dimensionless variable $\hat{s} = ls$. Then $Q^{(0)}(s, \varphi) \equiv Q^{(0)}(\hat{s})$ and satisfies the equation

$$2\hat{s}^2 \frac{\partial^2 Q^{(0)}}{\partial \hat{s}^2} - \hat{s}Q^{(0)} = 0, \qquad (23')$$

the solution of which is

$$Q^{(0)}(\hat{s}) = (2\hat{s})^{1/2} K_1((2\hat{s})^{1/2}).$$

We denote the integral of $K^{(n)}(\hat{s}, R)$ with respect to R in (21) by

$$\int_0^\infty dR K^{(n)}(\hat{s}|R) = (-1)^n \frac{z^{2n}}{2n!} Q^{(n)}(\hat{s}),$$

where

$$z^2 = \lambda|g_{eff}|\pi v. \qquad (24)$$

Using the condition (22) and Eq. (23), we obtain

$$\frac{\hat{s}z^2}{l} Q^{(n-1)}(\hat{s}) = 2\hat{s} \frac{\partial^2 Q^{(n)}}{\partial \hat{s}^2} - Q^{(n)}. \qquad (25)$$

The expression for the mean value (19) can now be written in the form

$$w_\lambda = 1 - \frac{z^2}{l} \int_0^\infty \Phi(z, \hat{s}) Q^{(0)}(\hat{s}) d\hat{s}, \qquad (26)$$

where we have introduced in (26) the definition

$$\Phi(z, \hat{s}) = \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n}}{2n!} Q^{(n)}(\hat{s}). \qquad (27)$$

The function $\Phi(z, \hat{s})$ (27) satisfies according to (25) and (23') the equation

$$\frac{\hat{s}}{l}\Phi(z, \hat{s}) = \frac{\partial^2}{\partial z^2}\left\{ 2\hat{s}\frac{\partial^2 \Phi}{\partial \hat{s}^2} - \Phi \right\}. \qquad (28)$$

Using the last expression and (23') we easily verify that

$$\int_0^\infty \Phi(z, \hat{s}) Q^{(0)}(\hat{s}) d\hat{s} = -2\frac{\partial^2}{\partial z^2}\left(\frac{\partial \Phi(z, \hat{s})}{\partial \hat{s}} \right)_{\hat{s}=0}. \qquad (29)$$

[We took into account the fact that $Q^{(n\neq0)}(0) = 0.$]

Thus, substituting (29) in (26), we have

$$w_\lambda = 1 + 2z^2 \frac{\partial^2}{\partial z^2}\left(\frac{\partial \Phi(z, \hat{s})}{\partial \hat{s}} \right)_{\hat{s}=0}. \qquad (30)$$

The solution of (28) for $\Phi(z, \hat{s})$ is given in the Appendix.

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For w_λ we obtain the simple closed-form equation

$$w_\lambda = \lambda\Delta/\text{sh}^2(\lambda\Delta)^{1/2}, \quad \Delta = 2\pi|g_{eff}|\tau^{-1}. \tag{31}$$

Returning to (18), we obtain

$$w(A) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\exp\left(\frac{xA}{\Delta}\right)\frac{x\,dx}{\text{sh}^2 x^{1/2}}. \tag{32}$$

The possible representation in series form follows from (32) because of the zeros of $\sinh(x^{1/2})$ on the negative-x axis:

$$w(A) = \frac{4\pi^2}{\Delta}\sum_{n\geq 1}\left[\frac{|A|}{\Delta}n^2\pi^2 - 1\right]n^2\exp\left(-n^2\pi^2\frac{|A|}{\Delta}\right). \tag{33}$$

The representation reduces in principle to an expression of (33) in terms of the elliptic function $\vartheta_3[\exp(\pi^2|A|/\Delta)|0]$ and its derivatives.

Equation (33) yields the asymptotic behavior of $w(A)$ at large $|A|$:

$$w(A) \cong \frac{4\pi^4}{\Delta}\cdot\frac{|A|}{\Delta}\exp\left(-\frac{\pi^2|A|}{\Delta}\right), \quad |A|\gg\Delta. \tag{34}$$

The asymptotic expansion at small $|A|$ can be obtained directly from the integral (32) by the "steepest descent" method. At small $|A|/\Delta$ large values of x are significant. The saddle point lies at $x_0 = |A|/\Delta$. We get

$$w(A) = \frac{1}{\pi^{1/2}\Delta}\left(\frac{\Delta}{|A|}\right)^{1/2}\exp\left(-\frac{\Delta}{|A|}\right), \quad |A|\ll\Delta. \tag{35}$$

5. DISCUSSION OF RESULTS

We turn now to the equations of Sec. 3. To calculate the coefficient of the Curie law in the susceptibility (at $g_{eff} > 0$) we must calculate $\langle A\rangle$:

$$\langle A\rangle = -(\partial w_\lambda/\partial\lambda)_{\lambda=0} = \Delta/3.$$

Thus, the susceptibility in repulsion is, according to (10″),

$$\chi = \mu^2\nu(E_F)\Delta/3T. \tag{36}$$

Similarly, the magnetization (11) as $T \to 0$ is given by

$$M = \mu\nu(E_F)(2\mu H + {}^1\!/_3\Delta + 2T\ln 2). \tag{36'}$$

In *attraction*, according to (13) and (31), where $\lambda = 1/2T$, the magnetic susceptibility at low temperatures decreases exponentially:

$$\chi_{geff<0} \approx \pi\mu^2\nu(E_F)(\Delta/2T)\exp[-(2\Delta/T)^{1/2}].$$

We calculate here $M(H)$ for weak fields, in accord with (14) and (35):

$$M(H) = \frac{\mu\nu(E_F)}{\pi^{1/2}}\left(\frac{\Delta}{2\mu H}\right)^{1/2}\exp\left(-\frac{\Delta}{2\mu H}\right), \quad \Delta\gg\mu H. \tag{37}$$

An exponential decrease similar to (37) appears also in the distribution functions $\langle n(\xi)\rangle$ of the particle energies in (17') and (17″) for both attraction and repulsion.

The linear laws in the dependence of the electronic specific heat on the temperature, which play the principal role at the lowest temperatures, were already obtained by us in Sec. 3 and are determined by expressions (16') and (16″). Although the total dependences of any thermodynamic quantity in Sec. 3 on the temperature can be obtained with the aid of (33) numerically in all temperature ranges, we made no such calculations

for reasons which will be made clear presently.

From the foregoing, comparing the results obtained for repulsion interaction with the results of experiments[2] for the compounds mentioned above, we can state that qualitatively our reasoning leads to the right direction. Of course, there is no quantitative agreement, since in our case Eq. (36) for the low-temperature susceptibility yields inevitably the Curie law rather than the law $\chi \propto T^{-\alpha}$ (Ref. 2), where α changes from substance to substance. We believe the reasons for this discrepancy to be primarily the fact that the strong assumption made here, namely that the potential of the interaction between the electrons is short-range, does not take into account the specific Coulomb character of the potential.

This last circumstance is of no importance for the problem dealing with a single filament, inasmuch as according to (3) the "active" localized states are separated by very large distances, and the wave functions decrease over distances of the order of l. The situation is different in real quasi-one-dimensional materials, in which the individual filaments, while independent, are separated only by a distance of the order of the lattice constant a in the transverse direction. The effect of screening of the Coulomb forces (disregarding for the time being their specifics in the considered objects) come into play only at distances of the order of the Debye radius r_D:

$$r_D^{-2} \sim e^2\nu(E_F)a^{-2}.$$

We shall show that now we can no longer confine ourselves to the interaction of two electrons with opposite spins in one localized state, but must take into account the effects of the spatial correlation of the occupation numbers of different states. In fact, in accordance with (1), the energy scale of the significant localized states is

$$e^2\nu(E_F)/\tau \sim e^2/l.$$

Let us estimate the number of such levels ΔN in a volume in the form of a cylinder of radius r_D and of length l in the energy interval e^2/l. Then it turns out that

$$\Delta N = \frac{\nu(E_F)}{a^2}(r_D^2 l)\frac{e^2}{l} \sim 1.$$

The question of the role of spatial correlation calls, in particular, also for the study of the character of the screening in a system of localized electrons. On the whole, we regard this problem as very interesting and worthy of a separate study.

APPENDIX

We rewrite (28) in terms of the dimensionless variables $y = z/(2l)^{1/2}$:

$$s\Phi = \frac{\partial^2}{\partial y^2}\left[s\frac{\partial^2\Phi}{\partial s^2} - \frac{1}{2}\Phi\right]. \tag{A.1}$$

$\Phi(y,s)$ is defined as a function of y on the interval $(0,\infty)$ and, according to (26), does not increase as $y \to \infty$. The remaining boundary conditions are obtained from the series expansion (27) of $\Phi(y,s)$, assuming the latter to converge everywhere at real $y > 0$:

$$\Phi(y=0,s)=(2s)^{1/4}K_1((2s)^{1/4}),\qquad\text{(A.2)}$$

$$\Phi(y,s=0)=1.\qquad\text{(A.3)}$$

It is convenient to use the Laplace transform with respect to the variable y:

$$\Phi_\varkappa(s)=\int_0^\infty e^{-\varkappa y}\Phi(y,s)\,dy,\qquad \Phi(y,s)=\frac{1}{2\pi i}\int_{-i\infty+\delta}^{i\infty+\delta}e^{\varkappa y}\Phi_\varkappa(s)\,d\varkappa.$$

The solution of the equation for $\Phi_\varkappa(s)$, obtained from (A.1),

$$\frac{s}{\varkappa^2}\Phi_\varkappa=s\frac{\partial^2\Phi_\varkappa}{\partial s^2}-\frac{1}{2}\Phi_\varkappa,\qquad\text{(A.4)}$$

will be sought in the form of a contour integral

$$\Phi_\varkappa(s)=\int_C W(\zeta,\varkappa)e^{\zeta s}\,d\zeta.\qquad\text{(A.5)}$$

For the function $W(\zeta,\varkappa)$ we have, in turn, the equation

$$\frac{\partial}{\partial\zeta}\Big[\Big(\zeta^2-\frac{1}{\varkappa^2}\Big)W\Big]+\frac{1}{2}W=0.\qquad\text{(A.6)}$$

The solution of (A.6) is

$$W(\zeta,\varkappa)=\frac{A(\varkappa)}{\zeta^2-\varkappa^{-2}}\exp\Big\{-\frac{\varkappa}{4}[\ln(\zeta-\varkappa^{-1})-\ln(\zeta+\varkappa^{-1})]\Big\}.\qquad\text{(A.7)}$$

The choice of the contour C in (A.5) is determined by the condition that the function $[W(\zeta,\varkappa)e^{\zeta s}]_C$ vanish on the ends of the contour. Figure 5 shows the definition of the cuts in expression (A.7) and the choice of the contour C. For $\Phi_\varkappa(s)$ we easily obtain from (A.5)

$$\Phi_\varkappa(s)=-2iA(\varkappa)\exp\Big(-\frac{\varkappa\pi i}{4}\Big)\sin\frac{\varkappa\pi}{4}\exp\Big(-\frac{s}{\varkappa}\Big)$$
$$\times\int_0^\infty\frac{e^{-us}\,du}{u(u+2\varkappa^{-1})}\exp\Big\{-\frac{\varkappa}{4}[\ln(u+2\varkappa^{-1})-\ln u]\Big\}.$$

(The logarithms here have cuts at negative values of the argument.) We rewrite the boundary conditions (A.2) and (A.3) directly for the function $\Phi_\varkappa(s)$:

$$\Phi_{\varkappa\to\infty}(s)=\frac{(2s)^{1/4}}{\varkappa}K_1((2s)^{1/4}),\qquad\text{(A.2')}$$

$$\Phi_\varkappa(s=0)=1.\qquad\text{(A.3')}$$

The condition (A.3') defines completely the solution $\Phi_\varkappa(s)$, with (A.2') satisfied automatically:

$$\Phi_\varkappa(s)=\frac{\exp(-s/\varkappa)}{2\varkappa}\int_0^\infty\frac{\exp(-us)\,du}{u(u+2\varkappa^{-1})}\exp\Big[-\frac{\varkappa}{4}\ln\Big(1+\frac{2}{\varkappa u}\Big)\Big],\qquad\text{(A.8)}$$

$\Phi_\varkappa(s)$ is analytically continued from (A.8) everywhere at $\mathrm{Re}\,\varkappa>0$.

Thus,

$$\Phi(y,s)=\frac{1}{2\pi i}\int_{-i\infty+\delta}^{i\infty+\delta}e^{\varkappa y}\,d\varkappa\frac{e^{-s/\varkappa}}{2\varkappa}\int_0^\infty\frac{e^{-us}\,du}{u(u+2\varkappa^{-1})}\exp\Big[-\frac{\varkappa}{4}\ln\Big(1+\frac{2}{\varkappa u}\Big)\Big],$$

from which we get for the quantity in (30)

$$\frac{\partial^2}{\partial y^2}\Big(\frac{\partial\Phi(y,s)}{\partial s}\Big)_{s=0}$$
$$=-\frac{1}{4\pi i}\int_{-i\infty+\delta}^{i\infty+\delta}\frac{l(l+1)\,dl}{l+2}\int_0^\infty t\,dt\exp\Big\{tl\Big[y-\frac{1}{4}\ln\Big(1+\frac{2}{l}\Big)\Big]\Big\}.\qquad\text{(A.9)}$$
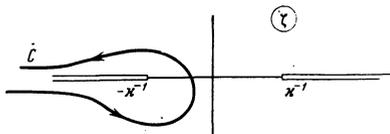
FIG. 5.

[On going from the preceding expression to (A.9) we first introduced the new variable $l=\varkappa u$, making use of the fact that $u<0$, and then made the substitution $t=u^{-1}$.]

Closing the contour of integration with respect to l in the left half-plane around the cut $(-2,0)$ and carrying out the integration in the converging integral with respect to t, we obtain

$$\frac{\partial^2}{\partial y^2}\Big(\frac{\partial\Phi(y,s)}{\partial s}\Big)_{s=0}=\frac{1}{4\pi i}\int_{C_1}\frac{(l+1)\,dl}{l(l+2)}\Big[y-\frac{1}{4}\ln\Big(1+\frac{2}{l}\Big)\Big]^{-2},$$

where the contour C_1 circles the cut $(-2,0)$ counterclockwise. Changing over in the last integral to the variable $\mu=l+1$ and integrating by parts, we transform the integral into

$$\frac{1}{2\pi i}\int_{C_1}d\mu\Big[y-\frac{1}{4}\ln\frac{\mu+1}{\mu-1}\Big]^{-1}.$$

This integral is written as a sum along the two "edges" of the cut and can be explicitly calculated with the aid of the residue theorem:

$$\frac{\partial^2}{\partial y^2}\Big(\frac{\partial\Phi(y,s)}{\partial s}\Big)_{s=0}=-\frac{1}{2y^2}+\frac{2}{\mathrm{sh}^2 2y}.$$

The substitution $y=z/(2l)^{1/2}$ and a definition of z in accordance with (24) lead to Eq. (31).

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[1] It can even be shown that this contribution is exactly equal to the correction to the susceptibility for the case of nonlocalized electrons.

[2] Of course, with all the stipulations made at the end of the preceding section concerning the applicability of these results at low temperatures.

[3] Thus, for example, [11]

$$c_V=T\Big[\Big(\frac{\partial S}{\partial T}\Big)_\mu-\frac{(\partial N/\partial T)_\mu^2}{(\partial N/\partial\mu)_T}\Big].$$

[4] We refer the reader to I for the definitions of most quantities employed below. We note, in particular, that the method in its general form, developed in I, can be equally well formulated in a representation that the defects or impurities occupy preferred positions in the lattice, or for a random Gaussian potential. Both approaches are perfectly equivalent for the reasoning that follows. Therefore, for example, in a number of cases we shall not distinguish between sums over the lattice and their continual representation in the form of integrals.

[5] We recall that in article I the potential of an individual impurity is in turn short-range.

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Translated by J. G. Adashko

Solitons and nonlinear resonance in two-dimensional lattices

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(Submitted 18 August 1979)
Zh. Eksp. Teor. Fiz. **78**, 831–840 (February 1980)

The behavior of solitary waves in two-dimensional lattices of nonlinear oscillators is investigated theoretically and experimentally. Solitons with an anisotropic relation between the amplitude and the duration are found. This anisotropy is preserved in the continual approximation. The proper "soliton modes" are studied in bounded lattices (resonators); it is shown that such modes are possible only for two configurations of the boundaries (rectangle and equilateral right triangle). The resonant excitation of soliton modes by a harmonic source (parametric generation of solitons) is considered. Experimental results of excitation of soliton modes in lattices of nonlinear electric oscillators are reported.

PACS numbers: 05.50. + q

INTRODUCTION

The role of solitary nonlinear waves—solitons—in lattice dynamics was recognized to be important quite long ago, starting with the attempts at interpretation of the known "paradox" of Fermi, Pasta, and Ulam,[1] which is connected with the anomalously slow stochastization in a system of nonlinear oscillators (we recall that the very term "soliton" was first introduced precisely in connection with this problem[2]). The properties of solitons in one-dimensional lattices (chains of coupled oscillators) were investigated in sufficient detail, and for particular forms of the interaction potential between the oscillators there are known solutions.[3] It was shown in addition that solitons can exist in multilayer semiconductor structures (superlattices),[4] as well as in multiband systems.[5] The role of soliton ensembles as collective excitations in lattices was investigated in a number of studies; conclusions were drawn that the solitons can contribute to the energy transport process that determines the thermal conductivity of crystals.[6] However, almost all the investigations were limited to one-dimensional processes. It is clear that both the properties of individual solitons and their collective behavior can be substantially different in two-dimensional and three-dimensional systems (see Ref. 6).

We consider in this paper solitons in two-dimensional lattices and investigate the resonant phenomena connected with the formation of "soliton modes" in bounded resonators of varying configurations. The theoretical analysis is based on the equations of a rectangular lattice of electromagnetic oscillators, for which the experimental results reported below were obtained. The conclusions, however, are more general in character and apply with practically no change, for example, to a corresponding system of mechanical oscillators.

THEORY

1. We consider a two-dimensional rectangular lattice consisting of identical elements and describable by the following nonlinear differential-difference equation:

$$L\frac{d^2 Q_{m,n}}{dt^2} = (u_{m-1,n} - 2u_{m,n} + u_{m+1,n}) + (u_{m,n-1} - 2u_{m,n} + u_{m,n+1}), \quad (1)$$

where $Q_{m,n}$ is a specified nonlinear function of $u_{m,n}$, and the subscripts are the coordinates of a given lattice site in its two dimensions.

Equation (1) corresponds directly to the oscillations of a lattice of electromagnetic oscillators, which was used in the experiment described below (Fig. 1), where L denotes the inductance of the element, $u_{m,n}$ the vol-
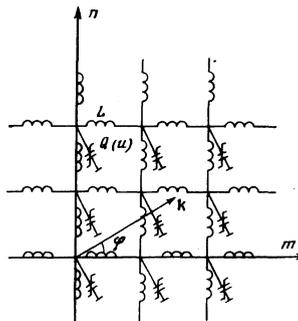
FIG. 1. Diagram of electric lattice used in the experiment.

0038-5646/80/020417-06$02.40