Anomalous behavior of electron scattering in a correlated system of charged donors

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This paper studies the anomalous behavior of the temperature dependence of the electron mobility μ in HgSe:Fe in the model of short-range correlations between charged donors that form resonance levels in the semiconductor. The calculations are done in the approximations of direct ion–ion correlations and quantum screening. The electron-mobility values obtained through calculations that do not use a single fitting parameter are found to be in good agreement with the experimental data in the 4.2–80 K temperature range for values of the iron content in the important $1.8\cdot 10^{19}$–$5.3\cdot 10^{20}$ cm^{-3} range. The $\mu(T)$ dependence is also calculated by the method of long-wave fluctuations of charged-donor concentration, where it is assumed that at fairly low temperatures long-range order sets in the system of such donors, that is, a Wigner crystal forms. Finally, it is demonstrated that calculations of $\mu(T)$ using this method with two fitting parameters yield results that agree qualitatively with the experimental data in a narrow low-temperature interval of 1.5–7 K and that the order-disorder transition temperature T_c can only be lower than 1 K.

1. INTRODUCTION

At low temperatures HgSe:Fe crystals exhibit a concentration "anomaly" in electron mobility: within a certain range of concentrations $N_{\rm Fe}$ of the impurity iron atoms the mobility μ increases with $N_{\rm Fe}$ (Refs. 1 and 2).[1)] To explain such anomalous behavior, Mycielski[3] suggested that the charged donors Fe^{3+} form a Wigner lattice (or a highly correlated liquid). The correlated positions of the donors result from the Coulomb repulsion between the donors, which tends to place the positive charges on the iron atoms that are the farthest away from each other. As a result of ordering of the charged impurity centers, electron scattering on these centers is weakened and the mobility increases in comparison to that in a crystal with randomly distributed impurities (say, HgSe:Ga). Mycielski's model seems attractive but, being an idealization of a real crystal with defects, cannot be used directly to interpret the experimental data, especially quantitatively. Here are the main drawbacks of the model.

1) Even for $T\to 0$ the lattice of charged donors has defects, since there is always a certain number of randomly distributed small donors in the sample, and in gapless semiconductors these donors are always ionized.

2) For HgSe:Fe crystals with $N_{\rm Fe^{3+}}\approx 5\cdot 10^{18}$ cm^{-3}, the average distance between Fe^{3+} ions, r_i, $\gtrsim r_s$ of the Coulomb potential. In such conditions screening weakens the interaction between ions and there is little possibility of a regular lattice of charged donors forming in the crystal.

3) The anomalous growth in μ with the increase in iron content $N_{\rm Fe}$ in HgSe begins at $N_{\rm Fe}\approx N^*_{\rm Fe}\equiv N_{\rm Fe^{3+}}\approx 5\cdot 10^{18}$ cm^{-3} (for $N_{\rm Fe}>N^*_{\rm Fe}$ the electron number density n is constant: $n=N^*_{\rm Fe}$), while strict periodicity in the system of Fe^{3+} ions leading to an increase in $\mu(N_{\rm Fe})$ can appear only as $N_{\rm Fe}/N_{\rm Fe^{3+}}\to\infty$.

Obviously, to describe the unusual behavior of $\mu(N_{\rm Fe})$ one must allow for the correlations in the spatial pattern of Fe^{3+} that are caused by ordering in the immediate vicinity of a given ion. Such calculations allowing for the Coulomb interaction between the nearest donors were recently done by Wilamowski *et al.*,[4] who described the degree of ordering in the system of ionized donors by a pair correlation function $g(r)$ approximated by a theta function, $g(r)=\theta(r-r_{\rm cor})$, where $r_{\rm cor}$ is the radius of the correlation sphere. After selecting the pair correlation function in this simple way, they calculated the electron-momentum relaxation time τ for scattering on ionized impurities and achieved rather good agreement between the calculated and experimental values of μ at $T=4.2$ K on the section of the $\mu(N_{\rm Fe})$ curve where $5\cdot 10^{18}\leqslant N_{\rm Fe}\leqslant 2\cdot 10^{19}$ cm^{-3}, that is, where Mycielski's model, based on the assumption that there is long-range order in a system of charged impurities, is invalid. This approach, however, does not allow a description of all the electronic properties of the HgSe:Fe system either. For instance, the results obtained in Ref. 4 predict that the $\mu(N_{\rm Fe})$ curve has a plateau at $N_{\rm Fe}>N^*_{\rm Fe}$, while the experimental data suggest that mobility actually decreases in this concentration range. Wilamowski *et al.*[4] were able to calculate the mobility and the Dingle temperature for only $T=4.2$ K. At the same time, the unusual temperature dependence of μ is obviously very important for establishing the reasons for the "anomalous" electronic properties of HgSe:Fe crystals.

Ablyazov and Èfros[5] have calculated the temperature dependence of μ for HgSe:Fe. They assumed that at fairly high temperatures (lower, however, than the energy of the Coulomb interaction of the Fe^{3+} ions, $e^2(N_{\rm Fe^{3+}})^{1/3}/\varkappa$, with $\varkappa$ the dielectric constant) the mobility value is limited by the vibrations of the Wigner lattice of charges and at low temperatures by the nonideality of the lattice caused by the random distribution of iron atoms. The idea of explaining the anomalous behavior of the temperature dependence of μ for $N_{\rm Fe}>N^*_{\rm Fe}$, that is, the sharp increase in electron mobility as the temperature drops (contrary to the predictions of the Brooks-Herring theory), suggested in Ref. 5, is interest-

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ing, but on the whole this approach and its realization contain essential faults. First, Ablyazov and Èfros assume that the set of charged donors Fe^{3+} forms a regular Wigner lattice. Second, in calculating the $\mu(T)$ dependence they used two fitting parameters, one of which is rather artificial since it must allow for the additionally introduced mechanism of electron scattering on neutral impurity centers, which, we believe, plays no important role in the conditions considered here. Besides, this fitting parameter strongly varies with the size of N_{Fe}, by more than a factor of ten in the $1\cdot 10^{19}$ to $1\cdot 10^{21}\ \mathrm{cm}^{-3}$ range.

We believe that to describe the system of iron ions with mixed valency in a self-contained manner it is expedient to employ methods used for systems with short-range order. Such methods have been developed in liquid state theory and proved useful, for one thing, in studying the electronic properties of liquid metals and melts. One of the most productive is the method of integral equations. In it one looks for the approximate integral equations that link the radial distribution function $g(r)$, which characterizes the spatial distribution of particles, with the interaction potential $U(r)$ between the particles. The method of integral equations makes it possible to establish the shape of $U(r)$ from the function $g(r)$ found from x-ray or neutron diffraction studies. Among the various nonlinear equations suggested by researchers the most exact is the Percus–Yevick equation.[6] An analytical solution in explicit form has been found only for a model in which the liquid is described by a set of hard spheres with the interatomic-interaction potential in the form

$$U(r)=\begin{cases}\infty, & r\leqslant d\\ 0, & r>d\end{cases}$$

where d is the diameter of a sphere. The use of this model can be justified by the fact that the results obtained with it are in good agreement with the results of numerical modeling by the Monte Carlo method. As shown by Ziman,[7] the structure and properties of liquids are determined primarily by the rapidly varying repulsive part of the potential, which with sufficient accuracy can be approximated by the hard-spheres potential. This suggests that the approach will also be fruitful in describing systems of charged donors, whose spatial correlation is ensured precisely by the Coulomb repulsive potential.

The expression derived by Percus and Yevick for the distribution function in the hard-spheres approximation does not contain the temperature explicitly; this function depends solely on the density of the system of particles. But then how is one to allow for the temperature? Several paths can be taken. We will discuss two that we believe most suitable for the HgSe:Fe system considered here.

2. THE APPROXIMATIONS OF DIRECT INTERIONIC CORRELATIONS AND QUANTUM SCREENING

The total distribution function[2)]

$$h(1,2)=g(1,2)-1, \tag{1}$$

which characterizes the correlation between atoms 1 and 2 (with coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$) caused by the acting forces, can be represented as the sumof two parts.[8] One, $c(1,2)$, describes the direct correlation between atoms 1 and 2; the other describes the indirect correlation emerging as a result of interaction with neighboring atoms, so that

$$h(1,2)=c(1,2)+N\int c(1.3)h(3.2)d3, \tag{2}$$

where N is the particle concentration.

The function $c(1,2)$ is nonzero only at small distances and depends primarily on the potential $U(1,2)$ of direct interatomic interaction, which falls off to zero over several interatomic distances. Therefore, for a fairly low concentration N the solution to Eq. (2) can be represented in the form of the Mayer function:

$$c(1,2)\approx \exp\left(-\frac{U(1,2)}{k_BT}\right)-1. \tag{3}$$

Approximation of $c(1,2)$ by the Mayer function (3) is valid for particle systems of moderate density, where the probability that the distance between atom 3 and atom 1 or 2 is smaller than the radius of potential $U(1,2)$ can be ignored. It is clear, therefore, that the structure factor

$$S(q)=1+4\pi N\int_0^\infty h(r)\frac{r\sin(qr)}{q}dr, \tag{4}$$

which enters into the expression for the electron-momentum relaxation time τ, is temperature dependent.

The relaxation time τ can be calculated by the formula for scattering on a system of ionized impurities:

$$\frac{1}{\tau}=\frac{2m(\varepsilon_F)}{3(2\pi\hbar)^3}\int_0^{2k_F}|V(q)|^2S(q)q^3\,dq, \tag{5}$$

where ε_F and $\hbar k_F$ are the Fermi energy and momentum, m the effective mass, and $V(q)$ the matrix element of potential U. This formula can be used to calculate $\mu = e\tau/m$ as a function of temperature for different values of the iron concentration N_{Fe}. This last quantity does not enter into Eq. (5) explicitly. It is easy to see, however, that both ε_F and k_F depend on N_{Fe}. Indeed, the electroneutrality equation

$$n=N_{\mathrm{Fe}}-N_{\mathrm{Fe}^{+2}}, \tag{6}$$

where $n=\int_0^\infty \rho_{\mathrm{con}}(\varepsilon)f(\varepsilon)d\varepsilon$ is the electron number density (ρ_{con} is the density of states in the conduction band, and f the Fermi distribution function), can be used to find ε_F. These calculations assume that the band parameters of the nonparabolic Kane band are the same as for HgSe. To calculate the number density of the donors occupied by electrons (i.e., neutral donors), $N_{\mathrm{Fe}^{2+}}=\int_0^\infty \rho_{\mathrm{Fe}}(\varepsilon)f(\varepsilon)d\varepsilon$, we must know the density of states ρ_{Fe}. Assuming that the ground state of iron donors is sufficiently sharp, we can put

$$\rho_{\mathrm{Fe}}(\varepsilon)=N_{\mathrm{Fe}}\delta(\varepsilon-\varepsilon_{\mathrm{Fe}}). \tag{7}$$

For high N_{Fe} present in HgSe samples formula (7) is a rather crude approximation since it does not allow for the natural and concentration broadening of a level or for Coulomb correlations between the charged donors. However, calculations that use a constant value of ρ_{Fe} in an interval of finite width (this requires introducing an additional unknown parameter, the level broadening) lead to practically the same results as formula (7).

Now let us consider the important problem of choosing the interaction potential $U(1,2)$. For the system of charged donors Fe^{3+} considered here it is natural to describe the interaction energy between the donors per donor via the screened Coulomb potential in the Thomas–Fermi approximation:

$$U_{\text{T-F}}(1,2)=\frac{e^2}{2\varkappa r_{12}}\exp\left(-\frac{r_{12}}{r_s}\right), \tag{8}$$

where $r_{1,2}\equiv|\mathbf{r}_1-\mathbf{r}_2|$.

Allowing for the fact that Eq. (8) provides an approximate representation of the true interaction between the Fe^{3+} ions and that the Mayer function (3) is also an approximation, we can attempt to "correct" the function (3) or the Thomas–Fermi potential via fitting parameters. Such parameters were introduced into the exponential and the pre-exponential factor in (8). It was found, however, that no values of the fitting parameters yield agreement between the calculated and experimental temperature dependences of the electron mobility μ. Not only is there no quantitative agreement; even qualitatively the theoretical and experimental $\mu(T)$ curves are different: one is convex, the other concave.

Note that the Mayer function (3) constitutes a rather good approximation for the function $c(1,2)$ since, as noted earlier, $r_s \lesssim r_i$, that is, the radius of the sphere within which $U(1,2)$ acts is of the order of, or less than, the average distance r_i between two ions, which means that a third ion does not enter the sphere.

As for the Thomas–Fermi approximation, it is clearly insufficient for the present case. This approximation is valid when the potential varies rather slowly in space, that is, for large wavelengths: $q\to 0$. For fairly small q, that is, $q\ll 1/r_i$, when the Thomas–Fermi approximation is valid, the Fourier transform of the screened potential (8) is

$$V_{\text{T-F}}(q)=\frac{4\pi e^2}{\varkappa(q^2+r_s^{-2})}. \tag{9}$$

For vectors q of the order of the inverse of the average interatomic distance, $q\sim 1/r_i$, the potential $U_{\text{T-F}}(r)$ cannot be thought of as slowly varying. Since in our problem the radius of the potential is fairly small, $r_s\lesssim r_i$, we must allow for the contribution of large values of q when calculating $V(q)$. This means that rather than the semiclassical Thomas–Fermi approximation one must use an expression given by the quantum screening theory in which the respective self-consistent Hartree equation is solved. Here neither the smallness of potential U, needed by the Thomas–Fermi equation to linearize the Poisson equation, nor the slow variation of U (this is achieved by allowing for the contribution of large q) is assumed. The solution to the Hartree equation is

$$V_H(q)=\frac{4\pi e^2}{\varkappa[q^2+r_s^{-2}G(q/2k_F)]}, \tag{10}$$

where

$$G\left(\frac{q}{2k_F}\right)=\frac{1}{2}+\frac{4k_F^2-q^2}{8k_Fq}\ln\left|\frac{2k_F+q}{2k_F-q}\right|.$$

In the long-wave limit, $V_H(q)$ and $V_{\text{T-F}}$ coincide: $V(q\to 0)=4\pi e^2/(\varkappa r_s^{-2})$.

If we represent (10) formally as (9), we can easily see that the effective screening length r_s is a function of q, growing with q, that is, the screening of the short-wave components of the potential ($q\to\infty$) steadily weakens. The potential $U(r)$ in the quantum screening theory (the Hartree potential) is specified by the following formula:[9]

$$U_H(\mathbf{r})=\frac{4\pi e^2}{\varkappa}\int\left\{q^2+\frac{6\pi e^2 n}{\varepsilon_F}\left[\frac{1}{2}+\frac{4k_F^2-q^2}{8qk_F}\times\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right]\right\}^{-1}e^{-i\mathbf{q}\mathbf{r}}d\mathbf{q}. \tag{11}$$

For small values of r this potential falls off faster than the potential (8), and for large values of r, owing to the singularity at $q=2k_F$, it contains an oscillating term proportional to $\cos(2k_Fr)$. In contrast to the Thomas–Fermi potential, the curve representing (11) intersects the axis of abscissas at a certain point $r=r_{\text{cr}}$.

Using potential (11) for calculating the relaxation time τ is difficult computationally. We, therefore, approximate (11) in the following manner:

$$U(r)=\begin{cases}U_{\text{T-F}}(r)-U_{\text{T-F}}(r_{cr}), & r\leqslant r_{cr}\\ 0, & r>r_{cr}\end{cases}. \tag{12}$$

For $r<r_{\text{cr}}$ this potential is smaller than (11) and tends to (11) as $r\to r_{\text{cr}}$. For $r>r_{\text{cr}}$ we have set $U(r)$ equal to zero since the amplitudes of the oscillations in (11) are very small and, according to (3), $c(1,2)$ tends to zero. Such an approximation appears reasonable because in the region where $r\sim r_{\text{cr}}$ and $(U/k_BT)<1$ potentials (11) and (12) differ little.

The interaction potential (12) is substituted into the Mayer function (3), which is used to calculate the structure factor $S(q)$. Of course, in (4) N must be replaced with the concentration of the trivalent ions, $N_{\mathrm{Fe}^{3+}}$. The upper limit of integration in (4) is set at $r_{\text{cr}}=0.6r_i$, since for $r_s<r_i$, the interaction between the closest Fe^{3+} ions is important. The value of r_{cr} at which $U(r)$ vanishes is calculated by formula (11).

After combining the Mayer function (3) with the chosen potential, we calculate the correlation radius r_{cor}. Figure 1 shows the temperature dependence of r_{cor} plotted as a result of our calculations. We see that r_{cor} decreases as the temperature rises. The correlation function $g(r)$ spreads out in this case near r_{cor}, that is, it differs from the step function corresponding to the hard-spheres approximation.

The physical meaning of the above approach to solving the problem of temperature dependence of the electron mobility is obvious. At finite values of t the electrons migrate between the Fe^{2+} and Fe^{3+} ions. As the temperature grows, the migration intensifies and, as Eq. (3) shows, the correlations between the charged Fe^{3+} donors weaken, the correlation radius r_{cor} decreases, the system of impurity ions Fe^{3+} becomes ever more random, the probability of electrons scattering on these ions rises, and μ drops. Here we can

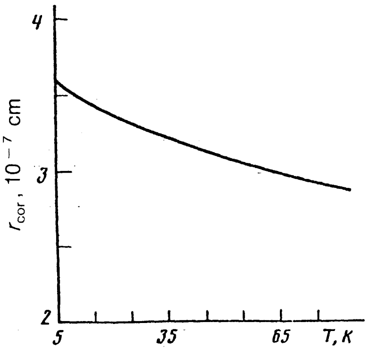

FIG. 1. Correlation radius versus temperature.

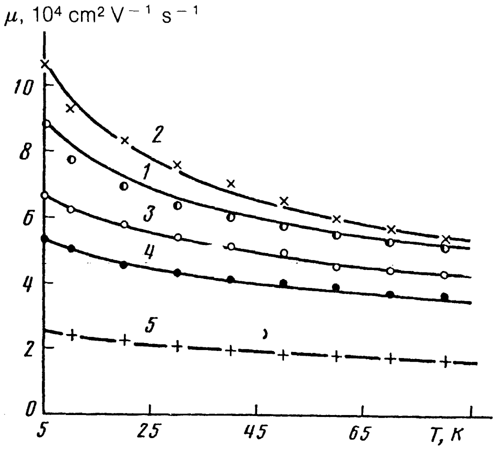

FIG. 3. The temperature curves representing the theoretical results (solid lines) and experimental data[10] for the electron mobility in HgSe:Fe samples with the following values of iron content $N_{\rm Fe}$ (cm^{-3}): (*1*) $8.8\cdot10^{18}$, (*2*) $1.8\cdot10^{19}$, (*3*) $8.8\cdot10^{19}$, (*4*) $1.8\cdot10^{20}$, and (*5*) $5.3\cdot10^{20}$. In accordance with Ref. 11, the phonon-scattering contribution has been subtracted from the experimental values of μ.

speak of a transition from the state of a correlated liquid to the gaseous state.

The decrease in μ with rising temperature follows directly from the expression for the relaxation time (5). Indeed, as t grows, the only function in the integral in (5) that is temperature dependent, $S(q)$, grows in the important range of q values, which follows directly from Eqs. (3) and (4) and is illustrated by Fig. 2, where $S(q)$ is depicted for two temperatures, 5 and 50 K, at $N_{\rm Fe} = 1.8\cdot10^{19}\,{\rm cm}^{-3}$. The value of S noticeably increases with temperature in the interval of values of q where the integrand of (5) has a maximum. Since $S(q)$ increases with T, the mobility drops, in accordance with (5).

The results of calculations of the temperature dependence of the electron mobility $\mu(T)$ with the iron content $N_{\rm Fe}$ varying between $8.8\cdot10^{18}$ and $5.3\cdot10^{20}\,{\rm cm}^{-3}$ are depicted in Fig. 3. Here we give the experimental values of μ taken from Ref. 10 from which the phonon-scattering contribution has been subtracted, following Ref. 11. In calculating $\mu(T)$ we used the following values of parameters: $n = N_{{\rm Fe}^{3+}} = 5\cdot10^{18}\,{\rm cm}^{-3}$, $\varkappa = 20$, $m = 0.07\,m_0$, $r_i = 5.8\cdot10^{-7}$ cm, and $r_s = 4.7\cdot10^{-7}$ cm. Figure 3 shows that the calculated mobility values are in good agreement with the experimental values for all $N_{\rm Fe}$. Comparison of the calculated curves representing $\mu(T)$ with the experimental curves from which the phononscattering contribution has not been subtracted can be done by analyzing Fig. 4 ($N_{\rm Fe} = 5.3\cdot10^{19}\,{\rm cm}^{-3}$). We see that for $T > 40$ K the calculated values of μ exceed the measured. This discrepancy suggests that phonon scattering contributes an ever growing amount as the temperature rises, a factor ignored in calculations.

The fact that the experimental data on $\mu(T)$ for samples with $N_{\rm Fe} > 1.8\cdot10^{19}\,{\rm cm}^{-3}$ practically coincide with the results of calculations that used no fitting parameters seemed incredible. But, faith in the results was strengthened by the discrepancy between experimental and calculated curves for $N_{\rm Fe} \leqslant 1.8\cdot10^{19}\,{\rm cm}^{-3}$. Matching calculation with the experimental data for $N_{\rm Fe} = 1.8\cdot10^{19}\,{\rm cm}^{-3}$ and $8.8\cdot10^{18}\,{\rm cm}^{-3}$ proved possible only by introducing the preexponential factors of 1.7 and 1.2, respectively, into the distribution function (3). The need for such "correction" of the Mayer function is due, apparently, to the fact that at relatively low iron content $N_{\rm Fe}$ when $N_{{\rm Fe}^{3+}}$ is only a fraction

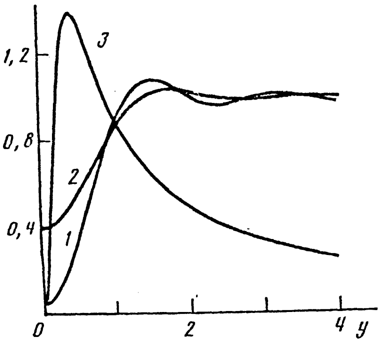

FIG. 2. The temperature dependence of the functions $S(q)$ (curve *1*, 5 K, and curve *2*, 50 K) and $F(y) = y^3/(y^2 + r_s^{-2})^2$ (curve *3*), with $y = q/2k_F$.

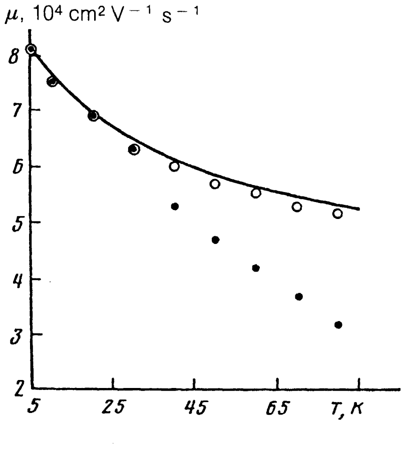

FIG. 4. The temperature curves representing the theoretical results (solid line) and experimental data[10] for the electron mobility in HgSe:Fe samples with $N_{\rm Fe} = 5.3\cdot10^{19}\,{\rm cm}^{-3}$. The experimental values of μ are depicted without the phonon contribution (○) and with the phonon contribution (●).

smaller than N_{Fe}, the correlation in the spatial distribution of charged donors is worse than for $N_{\mathrm{Fe}} \gg N_{\mathrm{Fe}^{3+}}$: the system of Fe^{3+} ions is more random. The difference in the fitting parameters for samples with $N_{\mathrm{Fe}} = 8.8 \cdot 10^{18}\ \mathrm{cm}^{-3}$ and $N_{\mathrm{Fe}} = 1.8 \cdot 10^{19}\ \mathrm{cm}^{-3}$ is most likely caused by the spread in the mobility values in the samples, which in view of the manufacturing technology should have had the same iron content. This is true not only of the region of low iron content but also of samples with $N_{\mathrm{Fe}} > 5.3 \cdot 10^{20}\ \mathrm{cm}^{-3}$, for which a large spread in values of μ (for samples that according to the manufacturing technology have the same value of N_{Fe}) is observed owing to the fact that a fraction of the iron atoms enters into the HgSe lattice as interstitial atoms rather than substitution atoms. To match the theoretical and measured values of μ in such samples a fitting parameter differing substantially from unity must be introduced in the pre-exponential factor in (3).

The obtained agreement between the calculated and experimental temperature curves for electron mobility for a broad range of concentrations of the iron impurity in HgSe may indicate that the model of short-range correlations that uses the modified Thomas–Fermi interionic interaction potential (11) and the correlation Mayer function (3) serves as an adequate approximation.

3. THE APPROXIMATION OF LONG-WAVE FLUCTUATIONS OF THE CHARGED-DONOR CONCENTRATION

The anomalous behavior of the temperature dependence of electron mobility was analyzed above in the short-range correlation approximation. The model of a Wigner crystal, which presupposes the existence of long-range order, was discarded on the grounds discussed in Sec. 1. Yet is clear that the model provides a qualitative explanation of the anomalous increase in μ as the temperature decreases: the lower the temperature, the rarer the hopping of electrons between the Fe^{3+} and Fe^{2+} ions, the system of ions Fe^{3+} becomes more and more ordered, and the scattering on this system weakens. Below we attempt to give a meaningful quantitative interpretation of the anomalies in the $\mu(T)$ dependence by assuming that at fairly low temperatures a transition of the "highly-correlated-liquid–Wigner-crystal" type in the system of ions Fe^{3+} becomes possible.

The theory of phase transitions states that long-wave fluctuations in the density of the medium increase near a transitions point. In our case these are fluctuations of the concentration of charged donors Fe^{3+} serving as scattering centers for electrons. The degree of ordering of a system of particles can be defined by a correlation function of the type

$$\Gamma(r) \propto \frac{1}{r} \exp\left(-\frac{r}{r_c}\right), \tag{13}$$

where r_{cor} is the correlation length, specifying the size of the ordering region. The temperature dependence of r_{cor} describes the variation in the degree of randomness of the system. At very high temperatures $r_{\mathrm{cor}} \to 0$, and the system is completely disordered. As the system is cooled, there first emerges short-range order (within one to two interatomic distances), and then r_{cor} becomes very large and characterizes critical fluctuations of concentration. When $r_{\mathrm{cor}} \to \infty$, long-range order sets in. The temperature at which this occurs is the order-disorder transition temperature.

In the vicinity of a phase transition point, where the scale of ordering in the system becomes large, long-wave fluctuations of the concentration of scattering centers must play the main role in the scattering of electrons. Information about variations in the number density of the system of particles can be obtained by studying the structure factor $S(q)$. In our situation the behavior of $S(q)$ for small values of the momentum transfer, $q = |\mathbf{k} - \mathbf{k}'|$, is essential (small-angle scattering). This distinguishes the scattering of electrons on long-wave fluctuations of concentration from scattering in the model of short-range fluctuations, according to which the fairly large values of momentum transfer, $q \sim k_F$, provide the main contribution to scattering [this follows directly from formula (5) for the relaxation time].

The limiting value $S(q)|_{q=0} = S(0)$ describes macroscopic variations in the density of the medium. In Eq. (4) the integral of the binary distribution function $g(\mathbf{r})$ can be interpreted as the ensemble average of the square of the number $\mathcal{N}$ of atoms in a given volume Ω:

$$\begin{aligned} S(0) &= 1 + N \int [g(\mathbf{r}) - 1]\, d\mathbf{r} \\ &= 1 + \frac{1}{\langle \mathcal{N} \rangle} \int [N(1,2) - N(1)N(2)]\, d1\, d2 \\ &= \frac{\langle \mathcal{N}^2 \rangle - \langle \mathcal{N} \rangle^2}{\langle \mathcal{N} \rangle}, \end{aligned} \tag{14}$$

where $N = \mathcal{N}/\Omega$.

Since the amplitude of the macroscopic-density fluctuations is proportional to the isothermal compressibility χ, for a thermodynamic system of the liquid or crystal type we have

$$S(0) = N k_B T \chi. \tag{15}$$

According to Landau's theory of phase transitions, in the vicinity of T_c compressibility grows sharply, $\chi \propto (T - T_c)^{-1}$ (see Ref. 12), and $S(0)$ becomes very large. The Fourier transform of the direct correlation function, $c(q)$, is related to the structure factor by the simple formula[7]

$$c(q) = 1 - 1/S(q) \tag{16}$$

and $c(0) \to 1$. Expanding $c(q)$ in the neighborhood of $q = 0$ in a power series in q^2, we get

$$c(q) = c(0) - r_0^2 q^2, \tag{17}$$

where the factor r_0 must be found. Substituting (17) into (16) and employing condition (15), we find that

$$S(q) = \frac{t}{r_0^2 (q^2 + r_c^{-2})}, \tag{18}$$

where $t = T/T_c$, and $r_{\mathrm{cor}}^2 = A r_0^2 |t - 1|^{-1}$, with A the fitting parameter in the theory. The main physical assumption made in deriving formula (18) is that r_0 is the parameter of local order in the medium and changes insignificantly even in the vicinity of the transition point.

The formula for the relaxation time τ in the case of electron scattering on long-wave fluctuations of density can be obtained by substituting the expression (18) for the structure factor into (5):

$$\frac{1}{\tau}=\frac{4\varepsilon_B\Phi}{3\pi\hbar},$$

$$\Phi=\frac{tb_0}{(b_c-b_s)}\left[\frac{b_c}{(b_c-b_s)}\ln\frac{b_c(1+b_s)}{b_s(1+b_c)}-\frac{1}{(1+b_s)}\right]. \tag{19}$$

ε_B is the Bohr energy,

$$b_0=(1/2k_Fr_0)^2,\quad b_s=(1/2k_Fr_s)^2,\quad b_c=b_0(t-1)/A.$$

Since we are considering scattering on long-wave fluctuations, that is, $q\ll 2k_F$, the temperature interval within which Eq. (19) is valid has an upper bound,

$$b_c=\frac{b_0|t-1|}{A}\ll 1, \tag{20}$$

while from below the validity of (19) is limited by the inapplicability of Landau's theory in the neighborhood of T_c.

As Eq. (19) shows, the theory contains three unknown parameters that must be found r_0, T_c, and A. Varying the parameters T_c and A, we tried to describe the experimental $\mu(T)$ curves for different values of iron content in HgSe:Fe. Parameter r_0 can be excluded from (19) by taking the ratio $\mu(T)/\mu(T_0)$, where T_0 was chosen equal to 4.2 K. The values of the main parameters such as $m(\varepsilon_F)$ and $N_{\mathrm{Fe}^{3+}}$ were chosen the same as in the method based on the direct-correlations and quantum-screening approximations, studied earlier in this paper.

It would seem that having two fitting parameters at our disposal offers great possibilities for matching the theoretical and experimental $\mu(T)$ curves. Analysis has shown, however, that for $T_c>4$ K no variation of parameters can make these theoretical and experimental curves match even qualitatively (curve *1* in Fig. 5). At $T_c=1$ K the calculated $\mu(T)$ curves for different iron content in HgSe:Fe are close to the results of measurement in a fairly narrow temperature interval, 1.5–7 K. But, unfortunately, at temperatures below 1 K mobility has been measured only at one point, $T=0.04$ K (Ref. 13), which does not permit comparative analysis of the results of calculations and measurements.

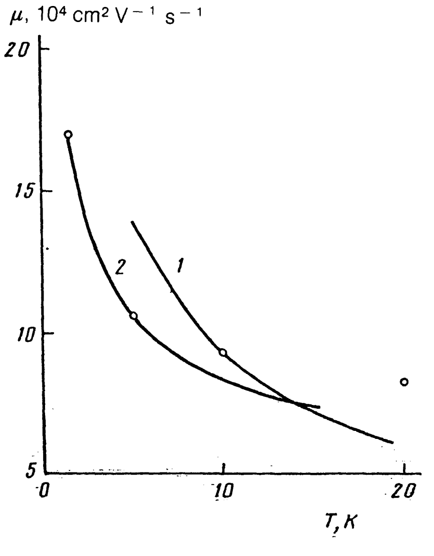

FIG. 5. The temperature curves representing the theoretical results (solid lines: curve *1*, $T_c=5$ K; curve *2*, $T_c=1$ K) and experimental data[10] for the electron mobility in HgSe:Fe samples with $N_{\mathrm{Fe}}=1.8\cdot 10^{19}$ cm^{-3} (Refs. 10 and 13). In accordance with Ref. 11, the phonon-scattering contribution has been subtracted from the experimental values of μ.

Comparing Figs. 5 and 3, we see that the $\mu(T)$ calculated by the short-range correlation method without introducing fitting parameters practically coincide with the measured values in the entire 4.2–80 K range, while the method of long-wave fluctuations of concentration does not allow achieving satisfactory agreement above 7 K for a single value of the fitting parameters. This firmly suggests that the model based on the assumption of long-range order in a system of charged donors (i.e., Wigner ordering of such donors) does not reflect the real situation with HgSe:Fe crystals. If ordering does emerge, it is only at temperatures below the transition temperature $T_c\sim 1$ K.

4. CONCLUSION

Summarizing, we must emphasize that the calculation method based on the model of short-range correlations between charged donors Fe^{3+} allows for a satisfactory quantitative explanation of the anomalous temperature behavior of the electron mobility in HgSe crystals alloyed with iron whose atoms form resonance donor levels. Calculation of the temperature dependence of μ by the method of long-wave fluctuations of the concentration of Fe^{3+} ions based on the assumption of long-range order in the system of these ions yields qualitative agreement with the experimental data only within a narrow temperature range of 1.5–7 K. It is safe to say that the assumption about the Wigner ordering in the system of Fe^{3+} ions does not agree with the experimental data on HgSe:Fe crystals. If ordering does appear, it is only for $T<T_c\sim 1$ K. Our attempts to calculate $\mu(T)$ at low temperatures by other means produced not only no quantitative but even no qualitative agreement. Thus, the model of short-range pair correlations, which made it possible to explain both the anomalous increase in electron mobility as the iron content in HgSe grows (see Refs. 2 and 4) and the anomalous temperature behavior of mobility, would seem to correctly reflect the nature of the interaction between the charge donors Fe^{3+} in HgSe:Fe and their role in electron scattering at low temperatures.

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1) Similar behavior of electron mobility has been discovered in HgSe:Cr crystals.[2]

2) The distribution function $g(r)$ has peaks at distances equal to the radii of the 1st, 2nd, etc. coordination spheres. As r increases, the peaks broaden, and for large r spread out completely against the background of the continuum, where $g(r)\to 1$. It is, therefore, often more convenient to reckon the distribution function from this background, that is, use the function $h(r)$.

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