Concentration anomaly in electron mobility in HgSe:Fe. A model of a highly correlated liquid

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This paper is a theoretical study of the unusual behavior discovered earlier of the dependence of the electron mobility μ in HgSe:Fe crystals on the iron concentration $N_{\rm Fe}$. We show that this anomalous behavior can be attributed to a combination of electron scattering by correlatively distributed charged donors $\rm Fe^{3+}$ and alloy scattering. We find that in the system of $\rm Fe^{3+}$ ions at low temperatures and at iron concentrations $(N_{\rm Fe} - N_{\rm Fe^{3+}})/N_{\rm Fe^{3+}} \ll 1$ the interionic Coulomb correlations are fairly weak, so that the system as a whole resembles a low-density gas. When $(N_{\rm Fe} - N_{\rm Fe^{3+}})/N_{\rm Fe^{3+}} > 1$, the Coulomb correlations are strong and the system of $\rm Fe^{3+}$ ions resembles a liquid.

1. INTRODUCTION

The model of short-range correlations has made it possible, on the qualitative level and sometimes even on the quantitative, to describe some anomalous electronic properties of HgSe crystals alloyed with iron, such as the temperature dependences of the electron mobility and of the Dingle temperature, the iron content in samples, and hydrostatic pressure.[1,2] All these features are caused by short-range order that sets in in the system of ionized iron impurities $\rm Fe^{3+}$. At the same time, the correlation model has thrown no light on the reason why the electron mobility μ decreases as the overall concentration of iron atoms $N_{\rm Fe}$ increases in the region where $N_{\rm Fe} \geqslant 2\times 10^{19}$ cm^{-3}. This decrease in μ seemed even more mysterious because up to $N_{\rm Fe} \geqslant 2\times 10^{20}$ cm^{-3} the mobility remains higher than in HgSe alloyed with shallow impurities, say, gallium. According to the correlation model, as $N_{\rm Fe}$ grows one should rather expect a weakening in the electron scattering on the impurity ions and an increase in mobility, since as the total concentration $N_{\rm Fe}$ of iron atoms increases with $N_{\rm Fe^{3+}}$ remaining constant, the ordering in the system of $\rm Fe^{3+}$ ions must increase and the system must more and more resemble a regular Wigner-like lattice.

The decrease in electron mobility μ in HgSe:Fe crystals with increasing iron content (Fig. 1) remained a mystery from the time it was discovered in 1985 (Ref. 3). It was assumed that this decrease in μ is related to effects of hybridization of donor d-states with band p-states. In the presence of hybridization the interionic interaction should weaken and the degree of ordering in the system of $\rm Fe^{3+}$ decrease. True, it is unclear beforehand how strongly the degree of ordering and, hence, mobility, must be decreased by hybridization as the overall concentration $N_{\rm Fe}$ increases.

References 1 and 2 analyze the role of effects of p–d hybridization and show that it is extremely weak. The broadening of the iron impurity level as a result of p–d hybridization is much smaller than the Coulomb interaction between $\rm Fe^{3+}$ ions. Hybridization, therefore, cannot disrupt the correlated distribution of the ionized donors and, hence, cannot lead to a decrease in mobility. Interdonor hybridization can likewise not cause $\mu(N_{\rm Fe})$ to decrease, since it is small due to the fairly strong localization of the d-states of iron. Our attempt to allow, in mobility calculations, for the broadening of the d-level of the iron atom due to interdonor hybridization led to results found to contradict the experimental data.

We have also analyzed the role of electron scattering on spin disorder associated with the exchange coupling of the spin of a band electron with the localized spin of an iron ion. Measurements of magnetic susceptibility suggest that the ground state of a $\rm Fe^{2+}$ ion in a tetrahedral crystal field constitutes a magnetic singlet, with the result that electron scattering with spin flip should play no role. The ground state of the $\rm Fe^{3+}$ ions is sixfold degenerate in spin, and scattering with spin flip is possible. But it is obvious that this process cannot be responsible for the decrease in $\mu(N_{\rm Fe})$ since the concentration of $\rm Fe^{3+}$ ions for $N_{\rm Fe} \geqslant 4.5\times 10^{18}$ cm^{-3} remains constant.

Below we present the results of a quantitative examination of the problem of how electron mobility is influenced by alloy scattering caused by the difference in potentials of the $\rm Hg^{2+}$ and $\rm Fe^{2+}$ ions that are substitution atoms in the HgSe lattice. The results of experiments suggest that only when $N_{\rm Fe} \geqslant 5\times 10^{20}$ cm^{-3} do the interstitial iron atoms act as additional sources of electron scattering. Neither alloy scattering nor the scattering on interstitial iron atoms, in contrast, say, to resonance scattering, disrupts the order in the spatial distribution of $\rm Fe^{3+}$ ions, and hence, neither has any marked effect on the increase in the electron mobility in HgSe:Fe as compared to HgSe:Ga.

As Fig. 1 shows, the mobilities μ in HgSe:Fe crystals exceed the values obtained through Brooks–Herring calculations up to $N_{\rm Fe} \approx 5\times 10^{20}$ cm^{-3} (the calculated values coincide with mobility values in HgSe crystals with shallow impurities, Ga and In). This means that the contribution of scattering on correlatively distributed charged donors $\rm Fe^{3+}$ is essential here.

On the basis of the model of short-range correlations, Wilamowski *et al.*[4] calculated the dependence of mobility μ on the iron content $N_{\rm Fe}$ for the section of the μ vs $N_{\rm Fe}$ curve (at $T = 0$) where μ increases.[1)] But their calculations correspond to the case of a weakly correlated collection of charged donors, whereas analysis shows (see below) that a system of $\rm Fe^{3+}$ ions constitutes a highly correlated Coulomb liquid, except for the range of exceptionally low iron content $[(N_{\rm Fe} - N_{\rm Fe^{3+}})/N_{\rm Fe^{3+}}] \ll 1$. Allowance for electron scattering on the correlated system of $\rm Fe^{3+}$ ions combined with

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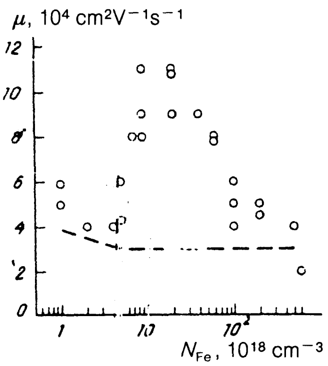

FIG. 1. Electron mobility in HgSe:Fe versus iron content; $T = 4.2$ K. The O correspond to the experimental data taken from Ref. 2, and the dashed curve corresponds indicates the results of Brooks–Herring calculations.

alloy scattering has enabled us to achieve good agreement of the calculated μ vs $N_{\rm Fe}$ dependence with the experimental data in the entire range of iron concentrations studied in experiments. The electron relaxation time τ for this situation can be written as $\tau^{-1} = \tau_c^{-1} + \tau_a^{-1}$, where τ_c and τ_a are relaxation times for scattering on correlatively distributed $\rm Fe^{3+}$ donors and for alloy scattering, respectively.

2. ELECTRON MOBILITY WITH ALLOWANCE FOR ALLOY SCATTERING

The relaxation time τ_c was calculated earlier by us[5,6] within the framework of the short-range correlation model and used to interpret the anomalous temperature dependence behavior of the mobility μ:

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

Here $m(\varepsilon_{\rm F})$ is the effective electron mass at the Fermi level, $\hbar k_{\rm F}$ the Fermi momentum, $V(q) = 4\pi e^2/\varkappa(q^2 + r_s^{-2})$ the Fourier transform of the scattering Coulomb potential $U(r)$, with $\varkappa$ the dielectric constant and r_s the screening length for the potential $U(r)$, and

$$S(q) = 1 + 4\pi N_{\rm Fe^{3+}} \int_0^\infty [g(r) - 1]\frac{r \sin qr}{q}\, dr, \tag{2}$$

is the structure factor, with $g(r)$ the pair correlation function.

In the case of a binary alloy, the product $|V(q)|^2 S(q)$ in Eq. (1) for the relaxation time must be replaced with (see Ref. 7)

$$\begin{aligned}&[N_{\rm Fe^{3+}}/N_{\rm Fe}]\,|V_+(q)|^2 S_{++}(q) + [N_{\rm Fe^{2+}}/N_{\rm Fe}]\,|V_0(q)|^2 S_{00}(q)\\ &\quad + 2[(N_{\rm Fe^{3+}} N_{\rm Fe^{2+}})^{1/2}/N_{\rm Fe}]\,|V_+(q) V_0(q)| S_{+0}(q).\end{aligned} \tag{3}$$

Here the subscripts "$+\,+$," "$+\,0$," and "00" signify that the respective quantities have been calculated for the $\rm Fe^{3+} - Fe^{3+}$, $\rm Fe^{3+} - Fe^{2+}$, and $\rm Fe^{2+} - Fe^{2+}$ interactions. Since the spatial distribution of the neutral donors $\rm Fe^{2+}$ is random, $S_{00}(q) = S_{+0}(q) = 1$. The relaxation time for alloy scattering can be represented as follows: $\tau_a^{-1} = \tau_{+0}^{-1} + \tau_{00}^{-1}$.

Let us write for $\tau_c \equiv \tau_{++}$, τ_{+0}, and τ_{00} the formulas that can be used to calculate the total relaxation time τ and the mobility $\mu = e\tau/m$:

$$\frac{1}{\tau_c} = \frac{2\pi\hbar N_{\rm Fe^{3+}}}{m a_B^2 k_F^3}\Phi_c,$$

$$\frac{1}{\tau_{+0}} = \frac{4(N_{\rm Fe^{3+}} N_{\rm Fe^{2+}})^{1/2}}{\hbar a_B k_F}\Phi_{+0} U_0, \qquad \frac{1}{\tau_{00}} = \frac{m k_F N_{\rm Fe^{2+}} U_0^2}{\pi\hbar^3}. \tag{4}$$

Here

$$\Phi_c = 2\int_0^1 \frac{x^3 S(2k_F x)\, dx}{(x^2 + b_s^{-2})^2}, \quad \Phi_{+0} = 1 - \frac{\ln(1 + b_s^2)}{b_s^2}, \quad b_s = 2k_F r_s,$$

with $a_{\rm B}$ the Bohr radius, $U_0 = \Omega\Delta U = \Omega\,(U_{\rm Hg^{2+}} - U_{\rm Fe^{2+}})$, and Ω the unit-cell volume. The quantity ΔU is the potential on which alloy scattering is realized and is the only unknown parameter of the theory. Estimates show that $\tau_{00}^{-1} \ll \tau_{++}^{-1}$.

Equations (4) imply that the ratio of the relaxation time τ_c/τ_{+0} is

$$\frac{\tau_c}{\tau_{+0}} = \Lambda\frac{\Phi_{+0}}{\Phi_c}\left[\frac{N_{\rm Fe^{2+}}}{N_{\rm Fe^{3+}}}\right]^{1/2}, \tag{5}$$

where the dimensionless parameter

$$\Lambda = \frac{m a_B k_F^2 U_0}{\pi\hbar^2} \tag{6}$$

is the ratio of the coupling constant for the interaction of electrons with neutral ($\rm Fe^{2+}$) and charged ($\rm Fe^{3+}$) donors.

According to Eqs. (4) and (5), the expression for the electron mobility as a function of iron content has the following form:

$$\begin{aligned}&\mu(N_{\rm Fe})\\ &= \mu_c\left\{1 + \frac{\Lambda}{2\Phi_c}\left(\frac{N_{\rm Fe}}{N_{\rm Fe^{3+}}} - 1\right)^{1/2}\left[4\Phi_{+0} + \Lambda\left(\frac{N_{\rm Fe}}{N_{\rm Fe^{3+}}} - 1\right)^{1/2}\right]\right\}^{-1}\end{aligned} \tag{7}$$

Here

$$\mu_c = \frac{e\tau_c}{m} = \mu_{BH}\Phi_{BH}/\Phi_c,$$

with $\mu_{\rm BH}$ the Brooks–Herring mobility for the scattering on a random system of impurity ions, and

$$\Phi_{BH} = \ln(1 + b_s^2) - b_s^2/(1 + b_s^2).$$

Formula (7) was used to calculate the dependence of electron mobility on the iron content. The parameter Λ and, hence, the potential ΔU of alloy scattering were found in two ways:

1. By varying the parameter Λ we ensured better agreement between the calculated and experimental μ vs $N_{\rm Fe}$ curves in the range where mobility decreases, that is, for $N_{\rm Fe} \geqslant 2\times 10^{19}$ cm^{-3}.

2. Near the peak observed on the μ vs $N_{\rm Fe}$ curve at $N_{\rm Fe} = N_m \simeq 2\times 10^{19}$ cm^{-3} the relaxation times τ_c and τ_a, describing the sections where mobility increases and decreases,

respectively, become equal, and from the condition that $\tau_{cm} \approx \tau_{am} = 2\tau_m$ the values of Λ and ΔU can be determined. Here τ_m is the total electron relaxation time due to both scattering mechanisms.

The following formula has been found for ΔU:

$$\Delta U = \frac{2\pi\hbar^2}{\Omega m a_B k_F^2}\left(\frac{N_{\mathrm{Fe}^{3+}}}{N_m - N_{\mathrm{Fe}^{3+}}}\right)^{1/2}\left[\left(1+\frac{\Phi_{cm}}{\Phi_{+0}^2}\right)^{1/2} - 1\right]\Phi_{+0}. \tag{8}$$

The value of $\Phi_{cm} = \Phi_{\mathrm{BH}}\,\mu_{\mathrm{BH}}/\mu_c = \Phi_{\mathrm{BH}}\mu_{\mathrm{BH}}/2\mu_m$ is determined from the experimental mobility at the maximum of the μ vs N_{Fe} curve, μ_m. Both ways of estimating ΔU give practically the same result, $\Delta U = 0.32 - 0.35$ eV.

By determining the coupling constant Λ of the interaction of electrons with neutral centers and employing the experimental value of the mobility, $\mu_{\exp}$, we can extract from the total mobility μ the part μ_c for which scattering on the correlated system of charged donors Fe^{3+} is responsible:

$$\mu(N_{\mathrm{Fe}}) = \mu_{BH}^{*}\left\{\frac{\mu_{BH}^{*}}{\mu_{\exp}} - \frac{\Lambda}{2\Phi_{BH}^{*}}\left(\frac{N_{\mathrm{Fe}}}{N_{\mathrm{Fe}^{3+}}} - 1\right)^{1/2}\right.$$
$$\left.\times\left[4\Phi_{+0} + \Lambda\left(\frac{N_{\mathrm{Fe}}}{N_{\mathrm{Fe}^{3+}}} - 1\right)^{1/2}\right]\right\}^{-1}, \tag{9}$$

where the asterisks denote quantities referring to $N_{\mathrm{Fe}}^{*} = 4.5\times10^{18}\ \mathrm{cm}^{-3}$ (at this value of iron content the electron number density n ceases to depend on N_{Fe}), $\mu_{\mathrm{BH}}^{*} \approx 3\times10^4$ $\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ and $\Phi_{\mathrm{BH}}^{*} \approx 2.2$. For $N_{\mathrm{Fe}} > N_m$ the value of μ_c reaches a plateau at $\mu_c \approx 2.3\times10^5\ \mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, which is μ_m, the peak value on the μ vs N_{Fe} curve.

Thus, the probability of scattering on a correlated system of charged donors proves to be smaller than on randomly distributed donors Fe^{3+} by a factor of seven or eight. An unlimited growth of $\mu(N_{\mathrm{Fe}})$, which must take place in the presence of long-range order in the system of Fe^{3+} ions, that is, when Wigner crystallization is realized, is impossible within the framework of the short-range correlation model, since in this model the growth of the correlation radius $r_c(N_{\mathrm{Fe}})$ is limited. To calculate $\mu(N_{\mathrm{Fe}})$ via Eq. (7) one must find the structure factor S, in terms of which the parameter Φ_c, is expressed, and the correlation function $h(r)$, on which S depends.

3. THE STRUCTURE FACTOR AND THE CORRELATION FUNCTION

For a meaningful description of the properties of a correlated system of Fe^{3+} in HgSe:Fe for $N_{\mathrm{Fe}} > N_{\mathrm{Fe}}^{*}$ we believe it expedient to resort to methods developed for systems with short-range order. Such methods have been developed in the theory of the liquid state. One of the most fruitful is that of integral equations. Within this method one seeks approximate integral equations linking the pair correlation function $g(1,2)$, which describes the spatial distribution of particles *1* and *2*, with the interaction potential $U(1, 2)$ between the particles. Ornstein and Zernick[8] represented the total correlation function

$$h(1,2) \equiv g(1,2) - 1 \tag{10}$$

as the sum of two parts. One, $C(1, 2)$, describes the direct correlation between particles *1* and *2*; the other the indirect correlation emerging as a result of interaction with neighboring particles, so that

$$h(1,2) = C(1,2) + N\int C(1,3)h(3,2)d3, \tag{11}$$

where N is the particle concentration; in the given case $N = N_{\mathrm{Fe}^{3+}}$.

The structure factor (2) can be expressed in terms of the Fourier transform of the total correlation function, $h(q)$, as follows:

$$S(q) = 1 + Nh(q) \approx \frac{1}{1 - NC(q)}. \tag{12}$$

3.1. Low particle concentrations. Weak interionic correlations

For a particle system of moderate density we can assume that the interaction potential $U(1, 2)$ falls off to zero over distances smaller than the average distance between particles. There is little probability that the distance between particle *3* and particle *1* or *2* is smaller than the radius of $U(1,2)$. Hence, at fairly low concentrations N we can ignore the integral term in Eq. (11) and approximate the solution by the Mayer function $f(1, 2)$:

$$C(1,2) \approx f(1,2) = \exp\left(-\frac{U(1,2)}{k_B T}\right) - 1. \tag{13}$$

For a rarefield gas the structure factor, in accordance with Eq. (12), is

$$S^{(0)}(q) = 1 + Nf(q), \tag{14}$$

where $f(q)$ is the Fourier transform of the Mayer function.

The approximation can be improved if we allow for the integral term in Eq. (11). Then

$$S^{(1)}(q) = \frac{1}{1 - Nf(q)}. \tag{15}$$

Obviously, (14) is the first term in the expansion of (15) in powers of N.

Let us now analyze the limits of applicability of the approximation accepted by Wilamowski *et al.*[4] in their calculations of the μ vs N_{Fe} dependence in the range where mobility increases. Choosing the pair correlation function $g(r)$ in the form of the unit step function

$$g(r) = \begin{cases} 0, & r < r_c, \\ 1, & r > r_c, \end{cases} \tag{16}$$

where r_c is the correlation radius, corresponds to the case of extremely low concentrations [see Eqs. (13) and (14)]. Here, essentially, a model is used in which the system of particles is described by a collection of hard spheres with diameter d with the following interaction potential between the particles:

$$U(r) = \begin{cases} \infty, & r \leqslant d, \\ 0, & r > d. \end{cases} \tag{17}$$

The correlation radius in (16) is equal to d.

As has been shown (see, e.g., Ref. 7), the structure and properties of liquids are basically determined by the rapidly varying repulsive part of the potential, which with sufficient accuracy can be approximated by the hard-spheres potential. This suggests that such an approach can also be fruitful in describing the system of charged donors in HgSe:Fe whose spatial correlation is ensured precisely by the Coulomb repulsive potential. As the iron content N_{Fe} increases, the electrons migrate between Fe^{2+} and Fe^{3+} ions, the system of Fe^{3+} ions becomes ever more ordered, and the correlation radius grows. We can say that the system of Fe^{3+} ions gradually transforms from the random "gaseous" state to a more ordered state, which is closer to a liquid. With N_{Fe} increasing, the probability increases that a third Fe^{3+} ion will find itself within a sphere whose radius is that of the interaction potential between particles *1* and *2*. Hence, when calculating $h(r)$ it is advisable to allow for the integral term in (11) and replace the Mayer function (13) with the Percus–Yevick function.[9]

As in the case of a liquid, it is convenient to introduce a packing factor $\eta = \pi d^3 N/6$ in terms of which the structure factor at $q = 0$ is expressed in the following manner:

$$S^{(0)}(0)=1-8\eta, \qquad S^{(1)}(0)=\frac{1}{1+8\eta}. \tag{18}$$

The approximation (16) for $g(r)$ accepted in Ref. 4, obviously, loses all physical meaning when $\eta > 1/8$, since in this case $S^{(0)}(0)$ is negative.

Let us write the equation that Wilamowski *et al.*[4] used to establish the link between the correlation radius r_c and the concentrations $N_{\mathrm{Fe}^{3+}}$ and N_{Fe},

$${}^4/_3\pi r_c^3 N_{\mathrm{Fe}^{3+}}=1-\exp[-{}^4/_3\pi r_c^3 N_{\mathrm{Fe}}]$$

in terms of the packing factor η:

$$\eta(N_{\mathrm{Fe}})=\frac{1}{8}\left[1-\exp\left(-8\eta\frac{N_{\mathrm{Fe}}}{N_{\mathrm{Fe}^{3+}}}\right)\right]. \tag{19}$$

For $N_{\mathrm{Fe}}/N_{\mathrm{Fe}^{3+}} \gg 1$ we have $\eta(N_{\mathrm{Fe}}) \to 1/8$. Equations (14), (15), and (18) imply that the calculations of Wilamowski *et al.*[4] are valid only for $\eta < 1/8$ and that the region where $\mu(N_{\mathrm{Fe}})$ is saturated lies outside the scope of their approximation. It is no wonder, therefore, that the mobility μ calculated in Ref. 4 increases approximately by a factor of 2.5, i.e., μ_c/μ_{BH} as N_{Fe} grows from N_{Fe}^* to N_m, while for the measured values the mobility ratio $\mu_m/\mu_{\mathrm{BH}}^*$ is approximately equal to four, and after we deduct the contribution of the alloy scattering for the region where $\mu(N_{\mathrm{Fe}})$ is saturated we get $\mu_c/\mu_{\mathrm{BH}} \approx 7$–8. This means that the approximation of a low-density system of particles or, which is the same, of weak interionic correlations, is truly inadequate for interpreting the μ vs N_{Fe} dependence observed in experiments in the entire range of iron content values N_{Fe}.

Thus, calculations that use the unit-step correlation function $g(r)$ correspond to the case of a rarefied, weakly correlated gas of Fe^{3+} ions and can be used only to interpret the very first section of the μ vs N_{Fe} where mobility increases. To calculate the μ vs N_{Fe} dependence in the entire range of N_{Fe} we must consider the case of high density of the system of particles, where the correlations between these are strong.

3.2. High particle concentrations. Strong interionic correlations

Of the three currently known methods for calculating pair correlation functions for highly correlated systems, the method of chains of Bogolyubov–Born–Green–Kirkwood–Yvon equations, the hyperchain approximation, and the Percus–Yevick approximation, the third has gained the widest success. Percus and Yevick[9] chose the direct correlation function $C(1, 2)$ in the form

$$C(1,2)\approx f(1,2)\exp\left(\frac{U(1,2)}{k_B T}\right)g(1,2). \tag{20}$$

Substitution of (20) and (11) leads to a closed equation for determining one of the functions, $C(1, 2)$ or $h(1, 2)$ or $g(1, 2)$. The strongest argument in favor of the Percus–Yevick approximation is that the results of calculations of the thermodynamic and kinetic properties of liquid metals and alloys are in good agreement with calculations by the Monte Carlo method for interaction potentials of various types (see Ref. 7). An important merit of this theory is the possibility of solving exactly the integral equations for $C(1, 2)$ in the hard-spheres approximation. The solution has the form

$$C(r)=\begin{cases}\alpha+\beta\left(\frac{r}{d}\right)+\gamma\left(\frac{r}{d}\right)^3, & r\leqslant d,\\ 0, & r>d.\end{cases} \tag{21}$$

Here

$$\alpha=\frac{(1+2\eta)^2}{(1-\eta)^4}, \qquad \beta=\frac{6\eta(1+0{,}5\eta)}{(1-\eta)^4}, \qquad \gamma=0{,}5\eta\alpha.$$

Substituting the function $C(1,2)$ of (20) into Eq. (11), we can build a series in powers of the particle concentration N and determine the magnitude and temperature dependence of the structure factor $S(q)$ of (12) for an arbitrary potential $U(r)$. In the first order in N we have

$$C^{(1)}(r)=f(r)+Nf(r)\int f(r')f(|\mathbf{r}-\mathbf{r}'|)\,dr'. \tag{22}$$

For the hard-spheres model, approximation (22) corresponds to (21) if in the latter we allow only for first-order terms in η. The exact function $C(r)$ for a dense liquid consisting of hard spheres constitutes a "smoothed-out" variant of the rectangular function $C^{(0)}(r) = f(r)$. It must be noted

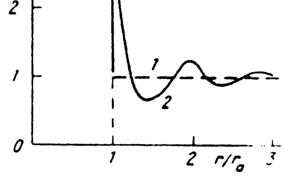

FIG. 2. The pair correlation function $g(r/r_a)$, where r_a $(N_{\mathrm{Fe}^{3+}})^{-1/3}$, in the hard-spheres approximation. Curve *1* corresponds to the limit of low particle concentration ($\eta < 0.125$), and curve *2* to the limit of high particle concentration ($\eta = 0.45$).

that for the modified Thomas–Fermi potential used in Refs. 5 and 6 to calculate the temperature dependence of mobility, the correlation function is close to the step function (16) corresponding to the hard-spheres approximation, where the interionic interaction potential U exceeds $k_B T$ considerably [$g(r)$ is exactly the step function as $T \to 0$]. Hence, our discussion of the μ vs $N_{\rm Fe}$ dependence in the case of high concentrations refers to the low-temperature range, where $U \gg k_B T$. Figure 2 depicts the pair correlation function $g(r)$ in the approximation specified by (16) (the unit step function) and in the approximation considered here.

If the Fourier transform of the direct correlation function $C(r)$,

$$C(q)=\frac{4\pi d^3}{u^3}\left\{\left[\alpha+2\beta+4\gamma-\frac{24\gamma}{u^2}\right]\sin u+\left[\frac{2}{u}(\beta+6\gamma)-(\alpha+\beta+\gamma)u-\frac{24\gamma}{u^3}\right]\cos u+\frac{24\gamma}{u^3}-\frac{2\beta}{u}\right\},\qquad u=dq, \tag{23}$$

is substituted into (12), we arrive at a formula for $S(q)$ valid for a dense, highly correlated system of particles.

4. ELECTRON MOBILITY WITH ALLOWANCE FOR STRONG INTERIONIC INTERACTION

Once we have obtained the expressions for the correlation function $C(r)$ and structure factor $S(q)$ and determined the magnitude of the scattering alloy potential ΔU, we can calculate the electron mobility μ as a function of iron content $N_{\rm Fe}$. It is worth noting that the value of Δ, estimated above by two methods employing the experimental values of mobility, can now, after we have calculated $C(r)$ and $S(q)$ for the cases of weak and strong interionic correlations, be evaluated without resorting to the experimental data, from the condition that the relaxation times τ_{cm} and τ_{am} are equal at the maximum of the μ vs $N_{\rm Fe}$ curve. Such calculations yield the same value $\Delta U \approx 0.35$ eV as given above.

To calculate $\mu(N_{\rm Fe})$ in the entire range of variations of $N_{\rm Fe}$ we must, obviously, know the contribution of mobility due to the scattering of electrons on the correlated system of charged donors, $\mu_c = \mu_{\rm BH}\Phi_{\rm BH}/\Phi_c$. If into Eq. (4) for Φ_c we substitute the expression (9) for $S(q)$ [or (12) combined with (23)], we find the dependence of Φ_c on the packing factor η. Hence, to calculate μ_c $(N_{\rm Fe})$ we must find the η vs $N_{\rm Fe}$ dependence.

Since Eq. (19) for $\eta(N_{\rm Fe})$ is valid only for $\eta < 1/8$, we are forced to turn to the experimental data on mobility. Using the measured value of mobility $\mu_{\rm expt}$ $(N'_{\rm Fe})$ for a certain concentration $N'_{\rm Fe}$, we determined, via Eq. (9), the value μ_c $(N'_{\rm Fe})$ and then built the μ_c vs η curve for $N'_{\rm Fe}$. Knowing for each concentration $N_{\rm Fe}$ the values of μ_c (η) found in this manner, we can easily determine the η vs $N_{\rm Fe}$ dependence. It was found that the ν vs $N_{\rm Fe}$ curves found from the experimental values $\mu_{\rm expt}$ are in good agreement with the η vs $N_{\rm Fe}$ curve calculated by an equation that generalizes Eq. (19) for the case of strong interionic interaction (Fig. 3):

$$\eta(N_{\rm Fe})=\eta_L\left[1-\exp\left(-\frac{\eta}{\eta_L}\frac{N_{\rm Fe}}{N_{\rm Fe^{3+}}}\right)\right], \tag{24}$$

where η_L is the packing factor for the liquid, $\eta_L \approx 0.45$. Figure 4 depicts the structure factor S plotted against the dimensionless parameter $q/2k_F$ (the curves were calculated in the approximations of weak and strong interionic correlations).

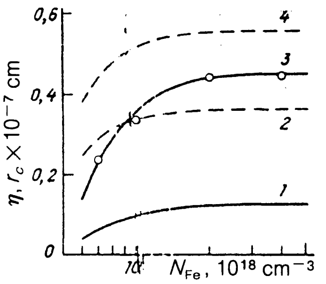

FIG. 3. The packing factor η (curves *1* and *3*) and the correlation radius r_c (curves *2* and *4*) as functions of iron content. Curves *1* and *2* correspond to the limit of low particle concentration ($\eta = 0.125$), and curves *3* and *4* to the limit of high particle concentration ($\eta = 0.45$); the O stand for the values of parameter η determined from the experiment.

In the limit of $N_{\rm Fe} \gg N_{\rm Fe^{3+}}$ the packing factor $\eta(N)$ tends to η_L. This suggests that when the iron content in HgSe is high, the system of $\rm Fe^{3+}$ ions at low temperatures is closer in its properties, determined by the correlation interaction, to a liquid rather than to a rarefied gas.

Once the η vs $N_{\rm Fe}$ dependence was found, we plotted μ_c and μ against $N_{\rm Fe}$ for the entire range of concentration of iron atoms in HgSe studied in experiments (Fig. 5). From Fig. 5 it follows that the agreement between the experimental data and the results of calculating the μ vs $N_{\rm Fe}$ dependence is satisfactory. The reader will recall that only one experimental parameter was used in the entire calculation, the value μ_m of mobility at the maximum of the μ vs $N_{\rm Fe}$ curve.

5. CONCLUSION

The good agreement of the calculations described above with the experiment may indicate that the basic mechanisms of electron scattering in HgSe:Fe at low temperatures $4.2 \leqslant T \leqslant 40$ K are the scattering on correlatively distributed charged ions $\rm Fe^{3+}$ and alloy scattering.

We have thus established that in the system of $\rm Fe^{3+}$ ions the interionic Coulomb correlations are fairly weak at low

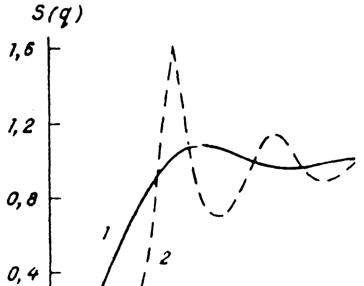

FIG. 4. $S(q)$ as a function of the dimensionless parameter $y = q/2k_F$. Curve *1* corresponds to the limit of low particle concentration ($\eta = 0.125$), and curve *3* to the limit of high particle concentration ($\eta = 0.45$).

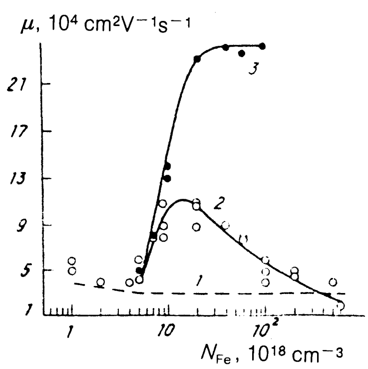

FIG. 5. Electron mobility as a function of iron content in HgSe:Fe ($T = 4.2$ K). The ● and ○ represent the experimental data of Ref. 2. Curve *1* corresponds to Brooks–Herring mobility calculations, curve *2* to mobility calculations that allow for alloy scattering and Coulomb correlations (the theoretical curve corresponds to $\Delta U = 0.35$ eV), and curve *3* to mobility calculations that allow only for interionic correlations.

temperatures and at $(N_{\mathrm{Fe}} - N_{\mathrm{Fe}^{3+}})/N_{\mathrm{Fe}^{3+}} \ll 1$ $(\eta \ll 1/8)$, so that on the whole the system resembles a low-density gas. For $(N_{\mathrm{Fe}} - N_{\mathrm{Fe}^{3+}})/N_{\mathrm{Fe}^{3+}} > 1$ $(\eta \approx 0.45)$ the Coulomb correlations are strong and the system of Fe^{3+} ions resembles a liquid. In the intermediate concentration range $(N_{\mathrm{Fe}} - N_{\mathrm{Fe}^{3+}})/N_{\mathrm{Fe}^{3+}} < 1$ $(0.125 < \eta < 0.3)$, the interionic correlations are not weak, but the properties of the system are far from those of a liquid. A nominal boundary between the regions of weak and strong correlations can be established if the limit value of the packing factor, $\eta = 1/8$, is used. At $\eta = 1/8$ the mobility μ_c calculated by the Percus–Yevick theory exceeds the value μ_{BH} of mobility calculated by the Brooks–Herring formula by a factor of two. Hence, the value $\mu_c/\mu_{\mathrm{BH}} \approx 2$ $(\mu_c \approx 6 \times 10^4\ \mathrm{cm}^2\ \mathrm{V}^{-1}\mathrm{s}^{-1})$ can serve for estimating the boundary value of N_{Fe} below which the weak-correlations approximation is valid. Estimates show that the boundary concentration is $N_{\mathrm{Fe}} \approx 5.5\text{–}6.0 \times 10^{18}\ \mathrm{cm}^{-3}$. At higher iron concentrations the results of Wilamowski *et al.*[4] cannot be used. Study of the region of strong Coulomb interionic correlations and simultaneous allowance for the contribution of alloy scattering have made it possible to describe quantitatively the μ vs N_{Fe} dependence in the entire range of iron impurity concentrations studied in experiments.

We note in conclusion that the transition from the region of strong correlations to that of weak correlations in the system of Fe^{3+} ions can be achieved by varying not only the value of iron content but the temperature as well. As the temperature rises, the correlations between the Fe^{3+} weaken, and for $T > 100$ K the system of ions transforms into a "gas."[5,6] The boundary value of the packing factor, $\eta = 1/8$ (or $\mu_c(T)\mu_{\mathrm{BH}} \approx 2$), enables finding the temperature at which the system goes from the strong-correlation range to the weak-correlation.

[1)] Other studies of the same authors, devoted to an analysis of the μ vs N_{Fe} dependence within the framework of the short-range correlation model, are cited in Refs. 1 and 2.

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