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Theory of Localized Electron States in an Isotropic Homopolar Crystal

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The behavior of an electron localized near a defect in a nonmetallic homopolar crystal is examined, taking into account the "condenson" interaction of the electron with the crystal. We have calculated the energy levels of the system and the energy of thermal dissociation of the electron, considering the motion of the electron quantum mechanically, and the motion of the atoms in the lattice either classically or quantum mechanically. It is shown that the condenson interaction leads to a difference between the energies of thermal and of photodissociation of an electron. We have determined the shape of the absorption band due to a localized electron (the position of the maximum, the halfwidth and its temperature dependence). As an illustration we give numerical calculations in the case of a Coulomb potential of the defect (for instance, an impurity atom with a valence electron).

1. INTRODUCTION

JUST as the presence of defects accompanied by localized electron states leads to the occurrence of a number of peculiarities in the optical, magnetic, photoelectric and other properties in ionic crystals, the presence of defects in homopolar crystals can also essentially change their properties.

It is well known that any attempt at a quantitative consideration of the energy level scheme of the electrons of an impurity atom leads to the calculation of the motion of a valence electron in the field of the ionized impurity in a medium characterized by a dielectric constant ϵ. We must at once remark that such a calculation which does not consider the interaction of the electron with the vibrations of the lattice is unable to consider quantitatively the width of the absorption band of impurity atoms, its temperature dependence, the difference between the energies of thermal and photodissociation, the difference between the energies of thermal and photo dissociation of impurity atoms, and so on.

In one of the papers[1] by the author and Pekar we investigated the question of the states of conduction electrons in a perfect homopolar crystal. It turned out that in a homopolar crystal also the interaction of the "extra" electron with the dielectric can partially be of an internal character. If as a result of an elastic deformation there occurs a region of increased density and thus a higher dielectric constant in some parts of the crystal, the electron must, according to macroscopic electrostatic theory, drift to those regions. Therefore, a region of higher density presents a potential trap to a conduction electron, and because of the inertia of the displacement of the atoms, it will not follow the motion of the electron.

If an electron localized in one of the discrete levels of such a trap is able to maintain such a region of higher density, this can lead to a self-adjustment of the electron state (as in the case of the polarons) and such a state we shall call a "condenson" in this paper. As a calculation showed, a condenson with a larger radius does not exist, and the macroscopic approximation for this solution therefore becomes illegitimate.

In Ref. 1 we gave only qualitative criteria for the existence of condensons. In the present paper we evaluate the energy levels and other parameters of the states of an electron localized near a defect in a homopolar crystal, taking into account the condenson interaction of the electron with the vibrations of the lattice. The calculation is given both semi-classically and by consistent quantum-mechanical methods.

It turns out that in the case considered the presence of a potential trap of a defect ensures the existence of localized states with a larger radius. Therefore, it is possible to make numerical calculations, using the macroscopic approximation and in particular to calculate the energies of thermal and photodissociation of an electron.

2. THE HAMILTONIAN OF THE SYSTEM

We calculate the behavior of an extra electron in a homopolar crystal with a defect. We denote the potential energy of the electron in the field of the defect by $Q(r)$.

As was shown in Ref. 1, the energy of interaction of an electron with an elastically deformed dielectirc (in the isotropic case and in the case of a cubic crystal) can be written in the macroscopic approximation in the form

$$V(r) = a(u_{11} + u_{22} + u_{33}). \qquad (1)$$

Here the expression in brackets is the trace of the deformation tensor, and a is the coupling constant.

The energy of the lattice vibrations can be written in the form

$$H_{\text{ac}} = H_{\|} + H_{\perp}. \qquad (2)$$

where $H_{\|}$ and $H_{\perp}$ are, respectively, the energies of the longitudinal and transverse vibrations. In the approximation we use here the electron interacts only with the longitudinal acoustic vibrations as follows from the considerations in Ref. 1.

The energy of these can be put in the form

$$H_{\|} = \frac{\rho}{2}\sum_{\varkappa}\dot{u}_{\varkappa}^{2} + \frac{1}{2}\left(K + \frac{4}{3}\mu\right)\sum_{\varkappa}u_{\varkappa}^{2}\varkappa^{2} \qquad (3)$$

where ρ is the density of the crystal, K and μ are the compressibility and shear moduli, $\varkappa$ is the wave vector, and $u_{\varkappa}$ the Fourier component of the displacement vector u in the expansion

$$\mathbf{u} = \sum_{\varkappa}\mathbf{u}_{\varkappa}\chi_{\varkappa}(r), \qquad (4)$$

$$\chi_{\varkappa}(r) = \sqrt{2/L^{3}}\begin{cases}\cos \boldsymbol{\varkappa}\mathbf{r}, & \varkappa_{x} \leqslant 0,\\ \sin \boldsymbol{\varkappa}\mathbf{r}, & \varkappa_{x} > 0,\end{cases} \qquad (5)$$

where L is the periodicity length of the crystal.

If we introduce normal coordinates by the equations

$$p_{\varkappa} = \dot{u}_{\varkappa}\sqrt{\rho/\hbar\omega_{\varkappa}}\ ; \quad q_{\varkappa} = u_{\varkappa}\sqrt{\rho\omega_{\varkappa}/\hbar}, \qquad (6)$$

where $\omega_{\varkappa} = v_{e}\varkappa$, while $v_{e} = [K+4/3\mu]^{1/2\ 1/2}\rho$ is the velocity of the longitudinal waves, (3) can be written in the form

$$H_{\|} = {}^{1}/_{2}\sum_{\varkappa}\hbar\omega_{\varkappa}(q_{\varkappa}^{2} + p_{\varkappa}^{2}). \qquad (7)$$

The transition to a quantum mechanical description of the motion of the atoms is accomplished by the substitution $p_{\varkappa} \to -i\partial/\partial q_{\varkappa}$.

The Hamiltonian of the system electron + defect + crystal can be written as follows:

$$\hat{H} = -(\hbar^{2}/2\mu_{0})\Delta + V(r) + Q(r) + \hat{H}_{\|}. \qquad (8)$$

Here we have already used the effective mass method[2], and μ_0 is the effective mass of the electron.

Considering Eq. (4), expression (1) for the interaction energy of the electron with the dielectric can be written in the form

$$V(r) = a\sum_{\varkappa}u_{\varkappa}\mid\varkappa\mid\chi_{-\varkappa}(r). \qquad (9)$$

We have finally for the Hamiltonian of the system.

$$\hat{H} = -(\hbar^{2}/2\mu_{0})\Delta + Q(r) + a\sum_{\varkappa}u_{\varkappa}\mid\varkappa\mid\chi_{-\varkappa}(r) + {}^{1}/_{2}\sum_{\varkappa}\hbar\omega_{\varkappa}(q_{\varkappa}^{2} - \partial^{2}/\partial q_{\varkappa}^{2}). \qquad (10)$$

The Hamiltonian of a free "condenson" can be obtained from (10) if we put $Q(r) = 0$.

The solution of the Schrödinger equation

$$\hat{H}\Psi = E\Psi \tag{11}$$

which corresponds to (10) determines the energy levels E and the wave functions of the system Ψ.

3. ENERGY LEVELS AND QUANTUM STATES OF THE SYSTEM IN THE SEMI-CLASSICAL APPROXIMATION. THE ENERGIES OF THERMAL AND PHOTODISSOCIATION OF AN IMPURITY CENTER.

By the semi-classical approximation we mean here that way of evaluating the behavior of the system in which the electron motion is calculated quantum mechanically, but the motion of the atoms in the lattice classically.

If we use the adiabatic approximation, the state of the system can be evaluated in two stages: first of all, the configuration of the medium (determined by the coordinates $u_\varkappa$) is supposed to be fixed, and the corresponding state of the electron is determined from the wave equation

$$\Big[-\frac{\hbar^2}{2\mu_0}\Delta + Q(r) + a\sum_{\varkappa} u_\varkappa |\varkappa| \chi_{-\varkappa}(r)\Big]\psi(r) = E\Big[u_\varkappa\Big]\psi(r). \tag{12}$$

After that we calculate the motion of the atoms (medium), the potential of which is supposed to be equal to

$$E[u_\varkappa] + U[u_\varkappa]. \tag{13}$$

For the adiabatic discussion mentioned a moment ago it is convenient to introduce the functional

$$\begin{aligned} F[\psi, u_\varkappa] &= (\hbar^2/2\mu_0)\int |\nabla\psi|^2 d\tau + \int Q(r)\,|\psi|^2 d\tau \\ &+ a\sum_{\varkappa} u_\varkappa\,|\varkappa|\int |\psi|^2\chi_{-\varkappa}(r)\,d\tau \\ &+ (\rho/2)\sum \omega_\varkappa^2 u_\varkappa^2. \end{aligned} \tag{14}$$

If in this functional all $u_\varkappa$ are kept fixed while its extremum is found with respect to ψ under the auxiliary condition

$$\int |\psi|^2 d\tau = 1, \tag{15}$$

then we get, in accordance with the quantum mechanical variational principle, the extremal function $\psi(r)$ as an eigenfunction of Eq. (12), but with the sum of the first three terms of (14) equal to $E[u_\varkappa]$. In that way, after the extremum with respect to ψ is found, $E[\psi, u_\varkappa]$ transforms into the potential energy of the atoms in the presence of a localized electron. The equilibrium configuration of the medium is in turn determined by the minimum of (13), and therefore the ground state of the system is determined by the absolute minimum of the functional (14) with respect to ψ and $u_\varkappa$.

The absolute minimum F can be found by first taking the variation with respect to $u_\varkappa$ and then with respect to ψ. In the result of the variation with respect to $u_\varkappa$ we have

$$u = -\frac{a}{|\varkappa|}K_{-\varkappa}\frac{1}{K + {}^4/_3\,\mu}, \tag{16}$$

$$K_{-\varkappa} = -\int |\psi|^2 \chi_{-\varkappa}(r)\,d\tau.$$

Substitution of (16) into (14) transforms F into a functional depending on ψ only,

$$J[\psi] = \frac{\hbar^2}{2\mu_0}\int |\nabla\psi|^2 d\tau + \int Q(r)\,|\psi|^2 d\tau - \frac{a^2}{2(K + {}^4/_3\mu)}\sum_{\varkappa} K_{-\varkappa}^2. \tag{17}$$

It is easily shown that

$$\sum_{\varkappa} K_{-\varkappa}^2 = \int \psi^4\,d\tau. \tag{18}$$

Hence,

$$J[\psi] = \frac{\hbar^2}{2\mu_0}\int |\nabla\psi|^2 d\tau + \int Q(r)\,|\psi|^2 d\tau - \frac{a^2}{2(K + {}^4/_3\,\mu)}\int \psi^4 d\tau. \tag{19}$$

Now we must find the minimum of J, taking the variation with respect to ψ. We obtain the minimum value of $J[\psi] - J[\psi_{1s}]$ and this will give us the energy of the thermal dissociation of a localized electron (if we neglect the small energy of a "free" condenson).

The Schrödinger level of the ground state (the energy of photodissociation) is determined from the relation

$$E_0 = \frac{\hbar^2}{2\mu_0}\int |\nabla\psi_{1s}|^2 d\tau + \int Q(r)\,|\psi_{1s}|^2 d\tau - \frac{a^2}{K + {}^4/_3\mu}\int \psi_{1s}^4 d\tau. \tag{20}$$

Hence, the difference between the energies of photo- and thermal-dissociation of a localized electron is found to be equal to

$$| E_0 - J | = \frac{a^2}{2(K + {}^4/_3\,\mu)} \int \psi_{1s}^4 \, d\tau. \qquad (21)$$

In that way also, in the case of homopolar crystals (as for ionic crystals), the energies of photo- and thermal dissociation are different, the energy of photo-dissociation being larger in absolute magnitude than the energy of thermal-dissociation.

It is possible to investigate the extremal properties of $J[\psi]$, if the actual shape of $Q(r)$ is given. We shall assume that $Q(r)$ is a Coulomb potential. This will, for instance, be the case, if we calculate the energy states of an impurity atom with a valence electron. In the macroscopic approximation the potential energy of a valence electron can is the effective charge of the ionized impurity. In that case (19) can be rewritten as follows,

$$J[\psi] = \frac{\hbar^2}{2\mu_0} \int | \nabla\psi |^2 \, d\tau - \frac{Ze^2}{\varepsilon} \times \int \frac{1}{r} | \psi |^2 \, d\tau - \frac{a^2}{2(K + {}^4/_3\,\mu)} \int \psi^4 \, d\tau. \qquad (22)$$

To investigate the extremal properties of (22), we treat it in the same way as was done in Ref. 1. We assume that there is a function leading to the minimum J. We introduce a function

$$\chi_0(r) = k^{3/2} \psi_0(kr). \qquad (23)$$

This function is normalized for $k > 0$, if $\psi_0(r)$ is normalized, and goes over into $\psi_0(r)$ for $k = 1$. Substituting (23) into (22), we get the following result:

$$J(k) = -a_1 k + a_2 k^2 - a_3 k^3, \qquad (24)$$

$$a_1 = \frac{Ze^2}{\varepsilon} \int \frac{1}{r} | \psi_0(r) |^2 \, d\tau;$$

$$a_2 = \frac{\hbar^2}{2\mu_0} \int | \nabla\psi_0(r) |^2 \, d\tau; \qquad (25)$$

$$a_3 = \frac{a^2}{2(K + {}^4/_3\,\mu)} \int | \psi_0(r) |^4 \, d\tau.$$

It follows from (24) that $J(k)$ is equal to zero for $k = 0$, then becomes negative, and reaches a minimum for $k = 1$ (provided $2a_2 = a_1 + 3a_3$), after that increases, passes through a maximum, and for still larger values of k decreases again. The full drawn curve in Fig. 1 shows J as a function of k. As $k \to \infty$, $J(k) \to -\infty$. As was noted in Ref. 1, this limiting behavior cannot be correct, as for $k \to \infty$ the effective radius of the electron r_e goes to zero so that the basis for the macroscopic approximation, for the method of effective masses, and so on, breaks down.

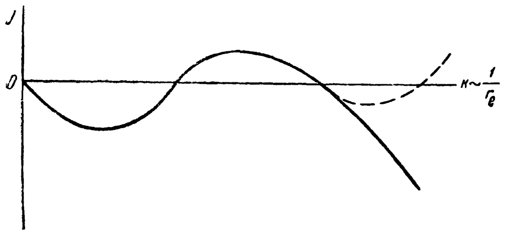

FIG. 1

However, in contradistinction to the case considered in Ref. 1, the functional of the system discussed here possesses a minimum, and this minimum occurs, generally speaking, for such a value of the effective radius r_e that the macroscopic and the other approximations used are still valid. Therefore, we can here discuss the problem quantitatively.

At the same time the qualitative discussion given in Ref. 1 shows that, if we generalize the functionals F and J to be applicable also for small values of the radius of the electron state, and taking, illegitimately, the limit $k \to \infty$ we are led to the conclusion that there may exist a minimum of condenson origin for those values of the radius.

Therefore, the most general functional of the system, valid for both small and large radii of the electron state, can, generally speaking, have two maxima (dotted curve in Fig. 1). In the framework of the variational method we can only attach any importance to the lowest of the two states.

Further, we shall only consider those crystals in which the first minimum lies more deeply than the second. The opposite case is apparently not very probable.

The minimum of the functional (22) can be found by straightforward variational methods. As a first qualitative approximation we choose a monotonically decreasing function without nodes,

$$\psi(r) = (\alpha^3 / 7\pi)^{1/2} (1 + \alpha r) e^{-\alpha r}. \qquad (26)$$

Substituting (26) into (22) we find a minimum

$J = J(\alpha)$, and using expression (21) we are able to determine the difference between the energies of thermal and photo-dissociation,

$$|E_0 - J| = 5.55\times 10^{-3} a^2 \alpha_m^3 / (K + {}^4/_3\mu), \qquad (27)$$

where α_m is the value of the parameter α corresponding to the minimum of J.

For an estimate of the size of the condenson effect we chose the values of the parameters nearly equal to the corresponding magnitudes for diamond and sulphur, namely, $\epsilon = 6$, $\mu_0 = m$, $K + 4/3\mu \approx 10^{11}$, $a = 2.5$, $Z = 1$. We then get $|E_0 - J| \approx 0.2$ ev. As can be seen from this estimate, the difference between the energies of thermal- and photo-dissociation can be shown to be considerable. In crystals with large ϵ, for instance, germanium or silicon, the values of J and E_0 are so small (hundredths of ev) that we can only hope to discover the difference in their magnitudes at very low temperatures.

4. OPTICAL PROPERTIES OF LOCALIZED CENTERS. QUANTUM MECHANICAL CALCULATION OF THE MOTION OF THE ATOMS

For a determination of the parameters of the absorption band of localized centers both the electron motion and the motion of the atoms in the lattice must be calculated quantum mechanically.

For an evaluation of the parameters of the ground state we take instead of (11) the equivalent variational functional[3],

$$\overline{H} = \int \Psi^* \hat{H} \Psi \, d\tau dq \qquad (28)$$

$$= \frac{h^2}{2\mu_0}\int |\nabla\Psi|^2 d\tau dq + \int Q(r)|\Psi|^2 d\tau dq$$

$$+ a\int \sum_{\varkappa} u_\varkappa |\varkappa| \chi_{-\varkappa}(r) |\Psi|^2 d\tau dq$$

$$+ \frac{1}{2}\sum_{\varkappa} \hbar\omega_\varkappa \int \Psi^* \left(q_\varkappa^2 - \frac{\partial^2}{\partial q_\varkappa^2}\right)\Psi d\tau dq$$

with the normalization condition

$$\int |\Psi|^2 d\tau dq = 1, \; d\tau = dxdydz, \qquad (29)$$

$$dq = dq_1 dq_2 \ldots dq_\varkappa \ldots$$

As in Ref. 3 we choose for the first approximation our function in the form

$$\Psi(r \ldots q_\varkappa \ldots) = \psi(r)\,\Phi(\ldots q_\varkappa \ldots). \qquad (30)$$

Substituting (30) into (28), using condition (29), and taking the variation with respect to Φ^* we get for Φ the equation

$$\Bigl(\sum_{\varkappa} H_\varkappa\Bigr)\Phi = \lambda\Phi, \qquad (31)$$

$$H_\varkappa = \frac{\hbar\omega_\varkappa}{2}\left[q_\varkappa^2 - \frac{\partial^2}{\partial q_\varkappa^2}\right] \qquad (32)$$

$$- \frac{a q_\varkappa}{\sqrt{(K + {}^4/_3\mu)}} K_{-\varkappa}\sqrt{\hbar\omega_\varkappa}.$$

Expression (32) can be rewritten in the following form:

$$H_\varkappa = \frac{\hbar\omega_\varkappa}{2}\left[(q_\varkappa - q_{\varkappa 0})^2 - \frac{\partial^2}{\partial q_\varkappa^2}\right] \qquad (33)$$

$$- \frac{a^2}{2(K + {}^4/_3\mu)} K_{-\varkappa}^2,$$

$$q_{\varkappa 0} = aK_{-\varkappa} / \sqrt{\hbar\omega_\varkappa (K + {}^4/_3\mu)}. \qquad (34)$$

Hence it follows immediately that Eq. (31) reduces to a set of oscillator equations,

$$H_\varkappa \Phi_\varkappa = \lambda_\varkappa \Phi_\varkappa, \qquad (35)$$

where $\Phi_\varkappa$ is an eigenfunction of the harmonic oscillator problem. The solution of (31) can be written in the form

$$\Phi = \prod_{\varkappa} \Phi_\varkappa, \; \lambda = \sum_{\varkappa} \hbar\omega_\varkappa\left(n_\varkappa + \frac{1}{2}\right) \qquad (36)$$

$$- \frac{a^2}{2(K + {}^4/_3\mu)} \sum_{\varkappa} K_{-\varkappa}^2.$$

Substituting (36) into (28), using condition (18) changes $\overline{H}$ into a functional depending on ψ only,

$$H_0[\psi] = \frac{\hbar^2}{2\mu_0}\int |\nabla\psi|^2 d\tau \qquad (37)$$

$$+ \int Q(r)|\psi|^2 d\tau - \frac{a^2}{2(K + {}^4/_3\mu)}\int \psi^4 d\tau$$

$$+ \sum_{\varkappa} \hbar\omega_\varkappa (n_\varkappa + {}^1/_2)$$

or, taking (19) into account,

$$\overline{H}_0 = J_0[\psi] + \sum_{\varkappa} \hbar\omega_\varkappa (n_\varkappa + {}^1/_2). \qquad (38)$$

This functional must be minimized with respect to ψ. Its extremal properties are determined by those of $J_0[\psi]$ which were examined in detail in the previous section. Thus we have, for instance, in the case of a defect potential of the form $Q(r) = Ze^2/\epsilon r$,

$$\overline{H}_0 = J_0(\alpha_{\mathrm{m}}) + \sum_{\varkappa} \hbar\omega_{\varkappa}(n_{\varkappa} + {}^1/_2). \qquad (39)$$

The calculation of the parameters of an excited state is analogous to the calculation of the parameters of the ground state.

Replacing Eq. (11) by the equivalent variational principle (28) and choosing as a first approximation the function in the form

$$\Psi_i = \varphi(r)\,\Phi(\ldots q'_{\varkappa}\ldots), \qquad (40)$$

we can obtain for the functional of an excited state after minimizing (with respect to Φ) the expression

$$\overline{H}_i = J_i(\varphi) + \sum_{\varkappa} \hbar\omega_{\varkappa}(n'_{\varkappa} + {}^1/_2). \qquad (41)$$

One can also find the minimum with respect to φ by straightforward variational methods once the form of $Q(r)$ is explicitly given. In particular, for $Q(r) = -Ze^2/\epsilon r$ it is plausible to choose φ in the form

$$\varphi = \pi^{-1/2}\beta^{5/2}e^{-\beta r}\,r\cos\vartheta. \qquad (42)$$

Substitution of (42) into (41) and finding the minimum determines β_{m} and $J_{i\mathrm{m}}$.

As Pekar and Krivoglaz[4] have shown, for localized centers of any structure in crystals with arbitrary dispersion laws for the eigenfrequencies of the lattice vibrations the position of the maximum of the absorption band is defined by the relation

$$\hbar\Omega_{\max} = |J_0 - J_i| = \hbar\sigma_1, \qquad (43)$$

$$\sigma_1 = \frac{1}{2}\sum_{\varkappa}(q_{\varkappa 0} - q_{\varkappa i})^2\,\omega_{\varkappa},$$

where $q_{\varkappa 0}$ and $q_{\varkappa i}$ are the coordinates of the equilibrium position of the system when the electron is respectively in the ground or in an excited state.

In the case of large energy release the halfwidth of the absorption curve is determined as follows:

1) high temperatures ($\hbar\omega_{\varkappa}/kT \ll 1$)

$$\vartheta = 4\sqrt{\ln 2}\,\sqrt{kT\hbar\sigma_1}; \qquad (44)$$

2) low temperatures ($\hbar\omega_{\varkappa}/kT \gg 1$)

$$\vartheta = 2\sqrt{2\ln 2}\,\hbar\sqrt{\sigma_2}\,; \qquad (45)$$

$$\sigma_2 = \frac{1}{2}\sum_{\varkappa}(q_{\varkappa 0} - q_{\varkappa i})^2\,\omega_{\varkappa}^2.$$

Substituting expression (34) for $q_{\varkappa 0}$ and $q_{\varkappa i}$ we have

$$\sigma_1 = \frac{1}{2}\,\frac{a^2}{(K + {}^4/_3\,\mu)\,\hbar}\sum_{\varkappa}(K_{-\varkappa 0} - K_{-\varkappa i})^2, \qquad (46)$$

$$\sigma_2 = \frac{1}{2}\,\frac{a^2}{(K + {}^4/_3\,\mu)\,\hbar}\sum_{\varkappa}(K_{-\varkappa 0} - K_{-\varkappa i})^2\,\omega_{\varkappa}.$$

The calculations lead to the following values of σ_1 and σ_2:

$$\sigma_1 = \frac{1}{2\pi}\,\frac{a^2}{\hbar\,(K + {}^4/_3\,\mu)}\,\alpha_{\mathrm{m}}^3\Big\{0.0348 - \frac{2}{7}\,\frac{[1 + 5v/(v+1) + v^3/2(v+1)^2}{(v+1)^5} + \frac{9}{256}\,\frac{1}{v^3}\Big\}, \qquad (47)$$

$$\sigma_2 = \frac{a^2}{2\hbar\sqrt{(K + {}^4/_3\,\mu)\,\rho}}\,\frac{\alpha_{\mathrm{m}}^4}{\pi^2}\Big\{0.107 + \frac{0.139}{v^4} - \frac{8}{7}\Big[\frac{-7v^8 - 480v^6 - 930v^4 - 32v^2 + 9}{6(v^2-1)^6} + \frac{2v^2\ln v}{(v^2-1)^7}(27v^6 + 141v^4 + 77v^2 - 5)\Big]\Big\},$$

where $V = \alpha_{\mathrm{m}}/\beta_{\mathrm{m}}$.

If we take $\epsilon = 6$, $\mu_0 = m$, $K + 4/3\mu = 10^{11}$, $a = 2.5$, the half-width of the absorption curve is equal to 0.1 ev at $T = 0$. Thus we are able to find, by determining the condenson interaction, a value for the halfwidth of the absorption curve even at the absolute zero.

The discussion of the condenson interaction of an electron of an impurity center with the lattice vibrations given here for a homopolar crystal must also be given for the cases of molecular or ionic crystals. In the latter case this interaction must lead to a deepening of the polaron level and a widening of the absorption band of the localized centers.

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