The author continues previous work (Uch. zap. KGU 55, 183, 1960) in which he studied the photo-ionization of an $F'$-center. Here the excited spectrum of an $F'$-center is calculated and the polaron wave function of this spectrum is derived more exactly than before. The Hamiltonian of the crystal in an effective-mass representation

$$\hat{H} = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) + u_1(r_1) + u_2(r_2) + u_{13}(r_{13}) + \sum_{x} A_x(r_x)q_x +$$

$$+ \sum_{x} A_x(r_x)q_x + \frac{\hbar^2}{2} \sum_{x} \left( q_x^2 - \frac{\partial^2}{\partial q_x^2} \right),$$

and the approximate wave function of the ground state, rewritten in variables of the polaron theory

$$\psi^0_{\omega}(\mathbf{r}_x) = \psi^0_{\omega}(\mathbf{r}_x) \prod_{x} \phi_{M_x}(q_x - r_{x'}).$$

(2)

Excited states of an $F'$-center

$$W_{\omega}^{\omega'}(\mathbf{r}_x, \mathbf{r}_x', \mathbf{k}) = W_{\omega}(\mathbf{r}_x)W_{\omega'}(\mathbf{r}_x')\psi_{\omega}(t) \prod_{x} \phi_{M_x}(q_x - r_{x'}).$$

(2)

(oc. ZhETF, 21, 11, 1951), are used to investigate the state of an $F'$ center in which one of the electrons is excited. $\psi_{\omega}(\mathbf{r})$ is the wave function of an electron localized in an $F'$ center and $\psi_{\omega}(\mathbf{r})$ is an approximate wave function, determined from the variation of

$$\overline{H}_z = \int \psi^*_\omega(t)\left[ -\frac{\hbar^2}{2M_0} + \frac{\hbar^2}{2} \sum_{x} (q_x^2 - q_{x'}^2) \right] \psi_\omega(t) \, dt.$$

(3)

$M_0$ is the polaron effective mass and $\phi_{M_x}$ are the wave functions of the harmonic oscillators of the lattice.
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$\hat{W}(r_1, r_2, q) = U_1(r_1) + U_2(r_2) + \sum A_n(r_1)(q_n - q_n') + \sum A_n(r_2)(q_n - q_n')$ \hspace{1cm} (6)

is taken as a perturbation operator. $q_{\xi}$ is the displacement of the equilibrium position of lattice oscillators, caused by an electron localized in the polarization potential well of a polaron, and $q_{\xi_0}$ is that caused by an electron localized in the $F'$ center. In zeroth approximation

$\psi_0^0(r_1, r_2) = \psi_0^0(r_1) \psi_p^0(r_2)$ \hspace{1cm} (10),

where $\psi_0^0$ and $\psi_p^0$ are the wave functions of electrons localized respectively in the polaron and in $F'$-center potential wells. These functions are considered as normalized ones. For the adiabatic potential

$F(q) = I_1 + I_2 - ce^2 \int \frac{\phi_0^0(r_1 - \xi) \psi_p^0(r_2)}{|r_1 - r_2|} + \frac{\hbar^2}{2M_0} \sum (q_n - q_n')^2$ \hspace{1cm} (16)

is obtained; $I_1$ and $I_2$ are the adiabatic potentials of $F'$-center and polaron. From the Schrödinger equation

$$-\frac{\hbar^2}{2M_0} \Delta \psi_\xi(t) + K(t) \psi_\xi(t) = E_{\xi_1...\xi_n} \psi_\xi(t)$$ \hspace{1cm} (23)

whose solution is the polaron wave function $\psi_\xi(t)$ and whose potential is given by

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$$K(\xi) = -\frac{e^{(3\xi^{2}-1)}}{(\xi^{2}-1)^{3}} \left( e^{-2\xi^{2}} - e^{-2\xi^4} \right) - \frac{e^{2\xi}}{4(\xi^{2}-1)^{3}} \left[ \gamma e^{-2\xi^{2}} + (2\xi^{2} - 1) e^{-2\xi^4} \right],$$  \hspace{1cm} (25)

$$\gamma = 1 + \frac{16}{5 \kappa c}.$$  \hspace{1cm} (26),

the discrete level of the polaron ground state is calculated, i.e. the variation of $E(\beta)$ is determined:

$$E(\beta) = \sum \int \varphi_{x}^{2}(\xi) \left[ -\frac{\hbar^{2}}{2M_0} \Delta_{x} + K(\xi) \right] \varphi_{x}^{2}(\xi) d\xi = \text{min}. \tag{28}$$

$$\frac{E(\beta)}{A} = \beta^{2} - 2A_{1}\beta^{2} \left[ \frac{1}{(\gamma^{2}+1)^{2}} - \frac{1}{(a_{1}+\beta)^{2}} \right] - \frac{2B\beta^{4}}{(a_{1}+\beta)^{4}} - \frac{2C\beta^{6}}{(a_{1}+\beta)^{6}}, \tag{29}$$

$$A_{1} = \frac{(3\gamma^{2}-1)\alpha_{1}}{(\gamma^{2}-1)^{3}}, \quad B = \frac{a_{1}^{2}(2\gamma^{2}-1)}{(a_{1}+\beta)^{4}}, \quad C = \frac{a_{1}^{4}}{(a_{1}+\beta)^{6}};$$

$$A = \frac{M_{p}^{2}}{2\hbar^{2}}, \quad a_{1} = \frac{5}{16} \kappa^{2}.$$  \hspace{1cm} (30)

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Excited states of an $F'$-center

$$\varphi_{0}(\xi) = \frac{\beta^{\xi}}{\sqrt{\pi}} \exp(-\beta \xi). \tag{27}.$$  \hspace{1cm} (27),

(29) is minimized numerically for NaCl ($\beta/a_{0} = 3.4$), KCl (3.0) and KBr (2.7) and for $E_{\beta} = -0.053$, -0.029 and -0.021 ev is obtained. For the potential energy

$$K(\xi) = \begin{cases} -K(\xi) \text{ for } \xi < \xi_{0}, \\ 0 \text{ for } \xi > \xi_{0}. \end{cases} \tag{32}$$

$$K(0) = \frac{5}{8} A \xi c \frac{(2\gamma^{2}-3\gamma^{4}+1)}{(1-1)(1-1)^{4}};$$

$$A = \frac{\mu \xi_{0}^{4}}{2\hbar^{4}}.$$  \hspace{1cm} (33)

with $\xi_{0} = 0.32 \AA$ (NaCl), 0.44 $\AA$ (KCl) and 0.73 $\AA$ (KBr) the following

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\[ K(0) = -0.11 \text{ ev (NaCl)}, \ -0.058 \text{ ev (KCl)} \text{ and } -0.051 \text{ ev (KBr)}. \]

For the continuous spectrum of a polaron in a square potential well

\[ K_o^2 = K^2 + \frac{2M_e}{\hbar^2} |K(0)| \]

for \( \langle \xi | \xi_0 \rangle \) and \( K = \left(2E_e M_e /\hbar^2 \right)^{1/2} \) for \( \langle \xi | \xi_0 \rangle \). There are

2 tables.