Here $V(\zeta_0) = V_1(\zeta_0) - V_2(\zeta_0)$; $V_1(\zeta_0)$ is the volume in momentum space occupied by the electrons; $V_2(\zeta_0)$ is the volume "occupied" by the "holes."

As is seen, μ_{xx} and μ_{yy} depend in this case on the angles between the field and the crystallographic axes and are determined exclusively by the energy spectrum. If the open surfaces are substantial[2], then μ_{xx} and μ_{yy} are functions of the angles. If $n_1 = n_2$ [hence $V(\zeta_0) = V_1(\zeta_0) - V_2(\zeta_0) = 0$ and $V'(\zeta_0) \neq 0$]*, then the asymptotic form of the tensor μ_{ik} is as follows: the $\mu_{\alpha\beta}$ increase linearly with the magnetic field ($\alpha, \beta = x, y$), and the μ_{iz} approach saturation. Hence, a study of the asymptotic form of the Thomson coefficient tensor in a strong magnetic field affords an additional possibility of investigating the topology of the equal-energy surfaces of the conduction electrons.

* There is no foundation for the assumption $V'(\zeta_0) = 0$. For example, in the case of a quadratic isotropic dependence:

$$V'(\zeta_0) = 2\pi (3V_{1,2}/4\pi)^{1/3} [(2m_1)^{1/2} + (2m_2)^{1/2}],$$

$m_1(m_2)$ is the effective mass of the electrons ("holes").

[1] A. H. Wilson, *The Theory of Metals*, Cambridge, 1954.
[2] Lifshitz, Azbel', and Kaganov, J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 220 (1956), **31**, 63 (1956); Soviet Phys. JETP **3**, 143 (1956), **4**, 41 (1957).
[3] M. Kohler, Ann. Phys. **6**, 18 (1949).
[4] L. Landau and E. Lifshitz, *Statistical Physics*, Moscow-Leningrad, Gostekhizdat, 1951.

Translated by M. D. Friedman
239

SOVIET PHYSICS JETP VOLUME 5, NUMBER 5 DECEMBER, 1957

Quantum States of Particles Coupled to a Harmonically Oscillating Continuum with Arbitrarily Strong Interaction, I. Case of Absence of Translational Symmetry

V. M. BUIMISTROV AND S. I. PEKAR
Physics Institute of the Ukrainian Academy of Sciences

(Submitted to JETP editor July 16, 1956)
J. Exptl. Theoret. Phys. (U.S.S.R.), **32**, 1193-1199 (May, 1957)

The ground-state energy is calculated by a variational method for the system defined by Hamiltonian (1). The trial wave-function is given by Eq. (3). The results are applied to the special cases of F and F'-centers. In the limits of weak and strong coupling, the calculated energy agrees with the exact results of second-order perturbation theory and of the adiabatic treatment respectively. The calculation can be regarded as an interpolation through the intermediate coupling region. It is valid when the effective size of the localized electron state is large, and when the conditions of the continuum model of F and F' centers are fulfilled.

WE CONSIDER systems described by a Hamiltonian of the form

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \Delta_i + \sum_{\varkappa, t} {}^1/_2 \hbar\omega_{\varkappa t} \left(q_{\varkappa t}^2 - \frac{\partial^2}{\partial q_{\varkappa t}^2}\right) + \sum_{\varkappa i t} c_{\varkappa t}^i q_{\varkappa t} \chi_{-\varkappa}(\mathbf{r}_i) + V(\mathbf{r}_1, \ldots, \mathbf{r}_N). \quad (1)$$

Here $\mathbf{r}_i$ is the radius-vector of the ith particle, m_i is its mass, $\omega_{\varkappa t}$ is the vibration frequency of the continuum corresponding to a wave-vector $\varkappa$ and to branch number t of the energy-surface, $q_{\varkappa t}$ is the normal coordinate of the same vibration, $c_{\varkappa t}^i$ is the coupling-constant between this vibration and the ith particle, $V(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the potential of the interaction of the particles with each other and with external fields, and

$$\chi_{+\varkappa}(\mathbf{r}_i) = \sqrt{\frac{2}{V}} \sin\left(\varkappa \mathbf{r}_i + \frac{\pi}{4}\right)$$
$$\varkappa_j = \frac{2\pi}{L} \nu_j; \quad j = 1, 2, 3; \quad (2)$$
$$\nu_j = 0 \pm 1, \pm 2, \ldots \quad V = L^3$$

Thus the $\chi_{+\varkappa}$ are a complete system of functions normalized in a volume V, comprising a cube of side L. In Eq. (1), the first term is the kinetic energy of the particles, the second is the energy of free vibration of the continuum, and the third is the interaction between particles and continuum. Such Hamiltonians occur in many physical situations. For example, the conduction electrons in a crystal have an interaction with the lattice vibrations which reduces to the form of Eq. (1) after the effective-mass approximation is made. The same is true of electrons localized around an impurity center, whose effect is included in the term $V(\mathbf{r}_1,\ldots,\mathbf{r}_N)$. The same type of Hamiltonian describes an exciton of large radius, in which the electron and hole move as two interacting quasi-particles. A similar Hamiltonian arises in the problem of a particle interacting with a quantized field.

The particular forms of $\omega_{\varkappa t}$, $c^i_{\varkappa t}$ and $V(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ will be chosen later when particular applications are considered. Initially we develop a general approximation method which applies to all values of these quantities. The energy levels will be calculated by a direct variational method which is valid for any strength of coupling. The results obtained go over, in the limits of weak and strong coupling, into the well-known results of perturbation theory and of strong-coupling theory. In this paper we consider the case of particles localized in a potential well produced by an external field. There is no translational symmetry. A following paper will deal with the case of translational symmetry.

I. CHOICE OF APPROXIMATE WAVE-FUNCTION AND DETERMINATION OF ITS VIBRATIONAL PART

One of the authors [1,2] showed earlier that the strong-coupling limit represents the particle as following adiabatically the comparatively slow oscillations of the continuum. The adiabatic approximation[3] consists in assuming for the system a wave-function of the form

$$\Psi = \psi(\mathbf{r}_i, q_{\varkappa t})\,\Phi(q_{\varkappa t}),$$

with ψ varying much slower than Φ as a function of $q_{\varkappa t}$. We showed further[1,2] that in $\psi(\mathbf{r}_i, q_{\varkappa t})$ one may replace the coordinates $q_{\varkappa t}$ by a self-consistent set of mean values, with an error which becomes smaller as the coupling becomes stronger. Consequently, as the coupling strength tends to infinity, the multiplicative approximation

$$\Psi = \psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\,\Phi(\ldots q_{\varkappa t}\ldots)$$

becomes exact. This is explained by observing that the particle moves so fast in its potential well that the slowly moving continuum feels only the average field of the ψ-cloud of the particle. Thus the continuum moves as if it were subjected to a given external force. The field of the ψ-cloud produces a displacement in the equilibrium positions of the continuum coordinates $q_{\varkappa t}$. The equilibrium values of these coordinates are functionals of ψ. If the coupling is weakened, the particle motion becomes slower and the continuum begins to feel the instantaneous field of the particle. Then the equilibrium positions $q^0_{\varkappa t}$ of the coordinates become functions of the particle positions $\mathbf{r}_i$, $q^0_{\varkappa t} = q^0_{\varkappa t}(\mathbf{r}_1\ldots\mathbf{r}_N)$. We thus approximate the wave-function of the system by the expression

$$\Psi = \psi(\mathbf{r})\prod_{\varkappa}\Phi_\varkappa(q'_\varkappa),\quad q'_\varkappa = q_\varkappa - q^0_\varkappa(\mathbf{r}), \tag{3}$$

where $\mathbf{r}$ denotes the totality of particle coordinates $\mathbf{r}_i$. We number the normal vibrations by a single index $\varkappa$ instead of the pair of indices $\varkappa, t$. The double indices can be reintroduced in the final results. The approximation (3) is a generalization of the multiplicative approximation mentioned earlier. We minimize the functional

$$\overline{H} = \int \Psi^* \hat{H}\Psi\, d\mathbf{r}\,dq,\quad dq = \prod_{\varkappa} dq_\varkappa$$

with the supplementary condition that Ψ be normalized. To do this we transform from the variables $\mathbf{r}_i\ldots q_\varkappa$ to the variables $\mathbf{r}_i\ldots q'_\varkappa$. The Jacobian of the transformation is unity. The energy-operator in terms of the new variables is

$$\hat{H} = -\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\Big[\Delta_i - 2\sum_{\varkappa}\Big(\nabla_i q^0_\varkappa,\ \nabla_i\frac{\partial}{\partial q'_\varkappa}\Big) + \sum_{\varkappa,\,\varkappa_1}(\nabla_i q^0_\varkappa,\ \nabla_i q^0_{\varkappa_1})\frac{\partial^2}{\partial q'_\varkappa \partial q'_{\varkappa_1}}$$
$$-\sum_{\varkappa}(\Delta_i q^0_\varkappa)\frac{\partial}{\partial q'_\varkappa}\Big] + \sum_{\varkappa}\frac{\hbar\omega_\varkappa}{2}\Big[(q^0_\varkappa + q'_\varkappa)^2 - \frac{\partial^2}{\partial q'^2_\varkappa}\Big] + \sum_{\varkappa i} c^i_\varkappa (q^0_\varkappa + q'_\varkappa)\chi_{-\varkappa}(\mathbf{r}_i) + V(\mathbf{r}). \tag{4}$$

Without loss of generality we may suppose that each of the functions ψ, $\Phi_\varkappa$ is normalized. We also suppose these functions to be real. Then, using the identity

$$\int \Phi_\varkappa \frac{\partial \Phi_\varkappa}{\partial q'_\varkappa} dq'_\varkappa = 0$$

and writing $\overline{\varphi} = \int \varphi(\mathbf{r}) |\psi(\mathbf{r})|^2 d\mathbf{r}$, we find

$$\begin{aligned} \overline{H}[\Psi] = &\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \int |\nabla_i \psi|^2 d\mathbf{r} + \sum_\varkappa \frac{\hbar\omega_\varkappa}{2} \overline{q_\varkappa^{02}} + \sum_{\varkappa i} c_\varkappa^i \overline{q_\varkappa^0(\mathbf{r}) \chi_{-\varkappa}(\mathbf{r}_i)} + \overline{V(\mathbf{r}_1, \ldots, \mathbf{r}_N)} \\ &+ \sum_\varkappa \frac{\hbar\omega_\varkappa}{2} \int \Phi_\varkappa \left(-\alpha_\varkappa \frac{\partial^2}{\partial q_\varkappa'^2} + q_\varkappa'^2 \right) \Phi_\varkappa dq'_\varkappa + \sum_\varkappa \hbar\omega_\varkappa \beta_\varkappa \int q'_\varkappa \Phi_\varkappa^2 dq'_\varkappa, \qquad (5) \\ &\alpha_\varkappa = 1 + \sum_i \frac{\hbar}{m_i \omega_\varkappa} \overline{(\nabla_i q_\varkappa^0)^2}, \quad \beta_\varkappa = \overline{q_\varkappa^0} + \frac{1}{\hbar\omega_\varkappa} \sum_i c_\varkappa^i \overline{\chi_{-\varkappa}(\mathbf{r}_i)}. \end{aligned}$$

We minimize this functional with respect to $\Phi_\varkappa$ for fixed ψ, and obtain the Euler equation

$$-\alpha_\varkappa (\partial^2 \Phi_\varkappa / \partial q_\varkappa'^2) + q_\varkappa'^2 \Phi_\varkappa + 2q'_\varkappa \beta_\varkappa \Phi_\varkappa = (2\lambda_\varkappa / \hbar\omega_\varkappa) \Phi_\varkappa.$$

Here $\lambda_\varkappa$ is a Lagrange multiplier introduced by the minimization. The Euler equation has the solution

$$\begin{aligned} &\Phi_\varkappa \equiv \Phi_{n_\varkappa} = A_{n_\varkappa} e^{-x_\varkappa^2/2} H_{n_\varkappa}(x_\varkappa), \quad \lambda_\varkappa \equiv \lambda_{n_\varkappa} = \frac{\hbar\omega_\varkappa}{2} [\alpha_\varkappa^{1/2} (2n_\varkappa + 1) - \beta_\varkappa^2], \qquad (6) \\ &x_\varkappa = \alpha_\varkappa^{-1/4} (q'_\varkappa + \beta_\varkappa), \end{aligned}$$

where $H_{n_\varkappa}$ is a Chebyshev-Hermite polynomial and $n_\varkappa = 0, 1, 2, \ldots$. Substitution of this result into Eq. (5) gives

$$\begin{aligned} \overline{H}[\Psi] = Q[\psi \ldots q_\varkappa^0] = &J[\psi] + \sum_\varkappa \hbar\omega_\varkappa (n_\varkappa + 1/2) + \sum_{\varkappa, i} \frac{\hbar^2}{2m_i} \overline{(\nabla_i q_\varkappa^0)^2} (n_\varkappa + 1/2) \\ &+ \sum_\varkappa 1/2 \hbar\omega_\varkappa (\overline{q_\varkappa^{02}} - \overline{q_\varkappa^0}^2) + \sum_{\varkappa, i} c_\varkappa^i [\overline{q_\varkappa^0 \chi_{-\varkappa}(\mathbf{r}_i)} - \overline{q_\varkappa^0}\, \overline{\chi_{-\varkappa}(\mathbf{r}_i)}], \qquad (7) \end{aligned}$$

$$J[\psi] \equiv \sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \int |\nabla_i \psi|^2 d\mathbf{r} - \sum_\varkappa \frac{1}{2\hbar\omega_\varkappa} \left(\sum_i c_\varkappa^i \overline{\chi_{-\varkappa}(\mathbf{r}_i)} \right)^2 + \overline{V(\mathbf{r})}. \qquad (8)$$

In deriving Eq. (7) we suppose that $q_\varkappa^0(\mathbf{r}) \sim V^{-1/2}$ and pass to the limit $V \to \infty$. In this case we can write

$$\alpha_\varkappa^{1/2} = 1 + \sum_i \frac{\hbar}{2m_i\omega_\varkappa} \overline{(\nabla_i q_\varkappa^0)^2}.$$

The functional (8) differs only in notation from the functional $J[\psi]$ appearing in the earlier papers, where the multiplicative approximation was used. See Eq. (29) of Ref. 2, or for F and F' centers Eqs. (23.11) and (26.10) of Ref. 1.

We shall next minimize the functional Q, varying $q_\varkappa^0(\mathbf{r})$ for fixed $\psi(\mathbf{r})$. The resulting Euler equation looks complicated and has not been solved in the general case. We solved it in the limits of weak and strong coupling and found that in both cases the solution can be written in the form

$$q_\varkappa^0 = \sum_i a_\varkappa^i \chi_{-\varkappa}(\mathbf{r}_i) \qquad (9)$$

with a suitable choice of the coefficients $a_\varkappa^i$. We

therefore use the approximation (9) for $q^0_\varkappa(\mathbf{r})$ in the general case, and use the variational method to determine the $a^i_\varkappa$. Substituting Eq. (9) into (7), we obtain

$$\begin{aligned} Q[\psi \ldots a^i_\varkappa \ldots] &= J[\psi] + \sum_\varkappa \hbar\omega_\varkappa (n_\varkappa + {}^1/_2) \\ &+ \sum_{\varkappa, i} \frac{\hbar^2}{2m_i}\, a^{i^2}_\varkappa \overline{[\nabla i\chi_{-\varkappa}(\mathbf{r}_i)]^2}(n_\varkappa + {}^1/_2) \\ &+ \sum_{\varkappa, i, i_1} \left[\frac{\hbar\omega_\varkappa}{2}\, a^i_\varkappa a^{i_1}_\varkappa + c^i_\varkappa a^{i_1}_\varkappa\right] \\ &\times \left[\overline{\chi_{-\varkappa}(\mathbf{r}_i)\chi_{-\varkappa}(\mathbf{r}_{i_1})} - \overline{\chi_{-\varkappa}(\mathbf{r}_i)}\;\overline{\chi_{-\varkappa}(\mathbf{r}_{i_1})}\right]. \end{aligned} \tag{10}$$

2. THE GROUND STATE

We obtain the energy of the ground state as the absolute minimum of the functional (10), in which we should set all $n_\varkappa = 0$ since this removes positive terms from the functional. The minimum is then found by a direct variational method.

If we take $\psi = \text{const} = V^{-1/2}$, which corresponds to the case $V(\mathbf{r}) = 0$ in the limit of weak coupling ($c^i_\varkappa \to 0$), then

$$\begin{aligned} &\overline{\chi_{-\varkappa}(\mathbf{r}_i)} = 0; \quad \overline{\chi_{-\varkappa}(\mathbf{r}_i)\chi_{-\varkappa}(\mathbf{r}_{i_1})} = \frac{\delta_{ii_1}}{V}, \\ &\overline{[\nabla i\chi_{-\varkappa}(\mathbf{r}_i)]^2} = \frac{\varkappa^2}{V}, \quad J[\psi] = 0. \end{aligned} \tag{11}$$

When Eq. (11) is substituted into (10) and the result is minimized with respect to the $a^i_\varkappa$, the ground-state energy becomes

$$E_0 = -\frac{1}{2V} \sum_{\varkappa, i=1}^{N} \frac{c^{i^2}_\varkappa}{(\hbar^2\varkappa^2/2m_i) + \hbar\omega_\varkappa}. \tag{12}$$

This coincides with the energy calculated by second-order perturbation theory. The last term in Eq. (1) is treated as the perturbation. In particular, in the polaron problem which has $N = 1$, $\omega_\varkappa = \omega$ independent of $\varkappa$, and

$$c^1_\varkappa = -e\sqrt{4\pi\hbar\omega c}/|\boldsymbol{\varkappa}|, \; c = 1/n^2 - 1/\varepsilon, \tag{13}$$

the energy is given by

$$E_{0p} = -\alpha\hbar\omega, \quad \alpha = e^2 c h^{-3/2}(m/2\omega)^{1/2}. \tag{14}$$

Here ε is the static dielectric constant of an ionic crystal, n is the refractive index, and m is the effective mass of a conduction electron in the crystal, assuming the ions to be fixed and motionless. Eq. (14) was obtained earlier by Fröhlich[4] using perturbation theory, and by Gurari[5] and Lee, Low and Pines[6] using variational methods.

From the other side, the approximation (3) also gives the correct ground-state energy in the strong-coupling limit, since even the less general multiplicative approximation, as we mentioned earlier, gives the right result in that limit. Knowing that the approximation (3) gives accurate results in both weak and strong coupling limits, we may hope that it also allows us to make a reasonable calculation in the intermediate coupling range.

In problems where $\psi(\mathbf{r})$ is symmetric in the particle coordinates, for example for the ground-state of an F'-center, and in various other cases, we may use for $\psi(\mathbf{r})$ the approximation

$$\psi(\mathbf{r}) = \prod_{i=1}^{N} \psi_i(\mathbf{r}_i) \tag{15}$$

If we also assume $\psi^2_i(\mathbf{r}_i) = \psi^2_i(-\mathbf{r}_i)$, we find

$$\begin{aligned} &\overline{[\nabla_i\chi_{-\varkappa}(\mathbf{r}_i)]^2} = \varkappa^2/V, \quad \overline{[\chi_{-\varkappa}(\mathbf{r}_i)]^2} \\ &= 1/V, \quad \overline{\chi_{-\varkappa}(\mathbf{r}_i)} = V^{-1/2}\,\overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i}. \end{aligned} \tag{16}$$

When these values are substituted into Eq. (10) and the result is minimized with respect to the $a^i_\varkappa$, we obtain

$$a^i_\varkappa = -\frac{c^i_\varkappa (1 - \overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i})}{(\hbar^2\varkappa^2/2m_i) + \hbar\omega_\varkappa (1 - \overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i})}, \tag{17}$$

$$Q = J[\psi] - \frac{1}{2V} \sum_{\varkappa i} \frac{c^{i^2}_\varkappa (1 - \overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i})^2}{(\hbar^2\varkappa^2/2m_i) + \hbar\omega_\varkappa (1 - \overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i})}. \tag{18}$$

In the subsequent calculations we must specify the form of the functions $\psi_i(\mathbf{r}_i)$. For many applications the following choice gives a good approximation:

$$\psi_i(\mathbf{r}_i) = (2\beta_i/\pi)^{3/4} \exp(-\beta_i\mathbf{r}_i^2). \tag{19}$$

In this case

$$\overline{\cos\boldsymbol{\varkappa}\mathbf{r}_i} = \exp(-\varkappa^2/8\beta_i)$$

and Eq. (18) gives (20)

$$Q = J[\psi] - \frac{1}{2V} \sum_{\varkappa, i} \frac{c^{i^2}_\varkappa (1 - \exp(-\varkappa^2/4\beta_i))^2}{(\hbar^2\varkappa^2/2m_i) + \hbar\omega_\varkappa (1 - \exp(-\varkappa^2/4\beta_i))}.$$

In the F-center problem there is only one electron ($N = 1$), $V = -ze^2/\varepsilon r$, $c_\varkappa$ is given by Eq. (13), and one may neglect the dispersion of longitudinal optical vibrations of the ions by setting $\omega_\varkappa = \omega$. Then, replacing sums by integrals according to the rule

$$\sum_{\varkappa} f(\varkappa) = (2\pi)^{-3} V \int f(\boldsymbol{\varkappa}) d\varkappa_1 d\varkappa_2 d\varkappa_3,$$

we obtain

$$Q_F = J(\beta) - \frac{2e^2 c V\sqrt{\beta}}{\pi} \int_0^\infty \frac{(1-e^{-x^2})^2\,dx}{bx^2 + 1 - e^{-x^2}},$$

$$x = \frac{\varkappa}{2\sqrt{\beta}}, \qquad b = \frac{2\beta\hbar}{m\omega}, \tag{21}$$

$$J(\beta) = \frac{3\hbar^2\beta}{2m} - \frac{e^2}{\sqrt{\pi}}\sqrt{\beta}\,(c + z2^{3/2}/\varepsilon). \tag{22}$$

The ground-state energy of the F-center is the minimum of Eq. (21) with respect to β.

In the strong-coupling limit we shall see that β is large. Thus $J(\beta)$, which contains terms of order β and $\beta^{1/2}$, is considerably larger than the second term in Eq. (21) which is of order $\beta^{-1/2}$. Hence the extremum of Q_F can be found approximately by minimizing the term $J(\beta)$ alone. This minimization was carried out in our earlier paper[7], with the result

$$\beta = (m^2e^4/9\pi\hbar^4)\,(c + 2^{3/2}z/\varepsilon)^2. \tag{23}$$

This value of β gives

$$E_F = -\frac{me^4}{6\pi\hbar^2}\left(c + \frac{2^{3/2}z}{\varepsilon}\right)^2 - \frac{2e^4mc\,(c + 2^{3/2}z/\varepsilon)}{3\hbar^2\pi^{3/2}} \int_0^\infty \frac{(1-e^{-x^2})^2 dx}{b_F x^2 + 1 - e^{-x^2}}, \tag{24}$$

$$b_F = (2me^4/9\pi\hbar^3\omega)\,(c + 2^{3/2}z/\varepsilon)^2.$$

In the denominator of the integrand in Eq. (24) we neglect $(1 - e^{-x^2})$ in comparison with the large term $b_F x^2$. The final result is then

$$E_F = -\frac{me^4}{6\pi\hbar^2}\left(c + \frac{2^{3/2}z}{\varepsilon}\right)^2 - 1{,}76\hbar\omega \Big/ \left(1 + \frac{2^{3/2}z}{\varepsilon c}\right). \tag{25}$$

We can go from the F-center to the polaron problem by setting $z = 0$. Eq. (24) then gives for the ground-state energy of the polaron

$$E_{0p} = -\frac{me^4c^2}{6\pi\hbar^2} - \frac{2e^4mc^2}{3\hbar^2\pi^{3/2}} \int_0^\infty \frac{(1-e^{-x^2})^2\,dx}{b_p x^2 + 1 - e^{-x^2}},$$

$$b_p = 2me^4c^2/9\pi\hbar^3\omega. \tag{26}$$

If here we neglect $(1 - e^{-x^2})$ compared with $b_p x^2$ in the denominator of the integrand, we obtain

$$E_{0p} = -(0.106\alpha^2 + 1.76)\,\hbar\omega. \tag{27}$$

This is the polaron ground-state energy in the strong-coupling limit.

It is interesting to see that Eq. (26) also gives the correct result (14) for the energy in the weak-coupling limit when β is small. The reason for this is that as $c \to 0$, $\beta \to 0$ too and hence $\psi \to$ const. A constant ψ, as we saw earlier, gives the perturbation-theory result. Hence Eq. (26) gives a single analytic expression for the polaron ground-state energy which is correct in both weak and strong coupling limits. It is reasonable to use it as an interpolation formula for the energy in the intermediate coupling region. But Eq. (26) was obtained from Eq. (21) by substituting the value of β from Eq. (23). This value of β was found by minimizing Eq. (21) in the strong-coupling limit. If we minimize Eq. (21) in the intermediate coupling range, we shall find a value of β differing from Eq. (23), and this will give a more accurate result (a lower value for E_{0p}) than Eq. (26).

A shortcoming of the approximations (3) and (19) as applied to the polaron problem is their lack of translational invariance. Only in the case of weak coupling, when ψ = const, is the correct translational symmetry preserved by the approximations. This shortcoming will be removed in a following paper, in which problems with translational symmetry will be considered separately and the correct approximations to use in such problems will be developed. We shall then find a lower value for the polaron ground-state energy.

The above criticism does not apply to problems of localized electron states where $V(\mathbf{r})$ contains a potential well binding the electron by means of external forces, for example the problems of F and F' centers, for in these cases there is no translational symmetry.

If we compare the formula (25) for the F-center ground-state energy with the corresponding result of the multiplicative approximation [8], we see that

the second term of Eq. (25) is new and is always negative. Thus our approximation (3) gives a lower ground-state energy. The lowering of the energy is particularly large for crystals with a high dielectric constant.

In the case of an F'-center there are two electrons ($N = 2$) attached to a positively charged crystal defect.

$$V = -\frac{ze^2}{\varepsilon}\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+\frac{e^2}{n^2|\mathbf{r}_1-\mathbf{r}_2|},$$

$$c_\varkappa^1 = c_\varkappa^2 = c_\varkappa,$$

and $c_\varkappa$ is given by Eq. (13). Then Eq. (20) gives

$$Q_{F'}(\beta) = J_{F'}(\beta) - \frac{4ce^2\sqrt{\beta}}{\pi}\int_0^\infty \frac{(1-e^{-x^2})^2\,dx}{bx^2+1-e^{-x^2}}, \quad (28)$$

$$J_{F'}(\beta) = \frac{3\beta\hbar^2}{m} - \frac{2e^2}{\sqrt{\pi}}\left(c'+\frac{2^{3/2}z}{\varepsilon}\right)\sqrt{\beta},$$

$$c' = 2c - \frac{1}{n^2}. \quad (29)$$

We minimize $Q_{F'}$ with respect to β by going to the strong-coupling range and minimizing only the main term $J_{F'}(\beta)$, just as we did for the F-center. This gives

$$\beta = (m^2e^4/9\pi\hbar^4)(c'+2^{3/2}z/\varepsilon)^2, \quad (30)$$

$$E_{F'} = -\frac{me^4}{3\pi\hbar^2}\left(c'+\frac{2^{3/2}z}{\varepsilon}\right)^2 - \frac{4ce^4m(c'+2^{3/2}z/\varepsilon)}{3\pi^{3/2}\hbar^2}\int_0^\infty \frac{(1-e^{-x^2})^2\,dx}{b_{F'}x^2+1-e^{-x^2}},$$

$$b_{F'} = 2me^4(c'+2^{3/2}z/\varepsilon)^2/9\pi\hbar^3\omega. \quad (31)$$

In the strong-coupling range we keep only the term $b_{F'}x^2$ in the denominator of the integrand, and obtain

$$E_{F'} = -\frac{me^4}{3\pi\hbar^2}\left(c'+\frac{2^{3/2}z}{\varepsilon}\right)^2 - \frac{3{,}52c\hbar\omega}{c'+2^{3/2}z/\varepsilon}. \quad (32)$$

This expression likewise differs from the result of the multiplicative approximation[9] only by the appearance of the second term on the right.

We have also studied the excited states of F-centers, for which the corrections to the results of the multiplicative approximation are significantly larger. These results were published elsewhere[10].

[1] S. I. Pekar, *Studies in the Electronic Theory of Crystals*, (Gostekhizdat, 1951), (German Translation, Akademie-Verlag, Berlin 1954).

[2] S. I. Pekar, J. Exptl. Theoret. Phys. (U.S.S.R.), **22**, 641 (1952).

[3] M. Born and J. R. Oppenheimer, Ann. Phys. **84**, 457 (1927).

[4] Fröhlich, Pelzer and Zienau, Phil. Mag. **41**, 221 (1950).

[5] M. Gurari, Phil. Mag. **44**, 329 (1953).

[6] Lee, Low and Pines, Phys. Rev. **90**, 297 (1953).

[7] S. I. Pekar and M. F. Deigen, J. Exptl. Theoret. Phys. (U.S.S.R.), **18**, 481 (1948).

[8] S. I. Pekar, J. Exptl. Theoret. Phys. (U.S.S.R.), **20**, 510 (1950).

[9] S. I. Pekar, and O. F. Tomasevich, J. Exptl. Theoret. Phys. (U.S.S.R.) **21**, 1218 (1951).

[10] V. M. Buimistrov and S. I. Pekar, Ukrain. Phys. Journ. **2**, 2 (1957).

Translated by F. J. Dyson
240