On the Lattice Polarization induced by Electronic Motion.

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§ 1. Introduction.

When an electron moves through the crystal lattice, the field of the electron induces the local electric polarization in the lattice, which polarization then affects in its turn the motion of the electron. Such reaction of the lattice polarization on the electronic motion has usually been taken into account when necessary by the introduction of the empirical dielectric constant into the theory\(^1\). In what kind of circumstance is such phenomenological treatment justified? In the following, we should like to give a partial answer to this question. The complete answer is no doubt only possible by a thorough quantum-mechanical treatment of the dielectricity of crystal lattices, which as far as we know, is not yet taken up by any investigators at the present time. In the present paper we have been able to enter into this important problem only superficially and we hope to come back again to the more detailed treatment of the subject.

In § 2 we give the method of the calculation of the polarization potential energy of an electron introduced into the ionic lattice, in § 3 we make some approximate calculations of this potential and discuss the trapping of an electron in a perfect ionic lattice, finally in § 4 we give some example of cases in which the usual theory with empirical dielectric constant does not work consistently.

§ 2. General Method of Calculation by Perturbation Theory

The Schrödinger equation of the system: an ionic lattice plus an additional electron is written as follows,

\[
\left( -\frac{\hbar^2}{2m} \Delta + H_e + H_v + \mathcal{V} + \mathcal{V}' \right) \Psi = -\frac{\hbar}{i} \frac{\partial \Psi}{\partial t},
\]

where the first term on the left hand side is the kinetic energy of the additional electron, \(H_e\) and \(H_v\) are electronic and vibrational energy of the crystal lattice respectively. The interaction energy of the additional electron and the lattice \(\mathcal{V}\) is composed from two parts, namely \(\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2\), where \(\mathcal{V}_1\) is the electrostatic interaction with crystal electrons and ions.
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\[ V_1 = \sum_i e^2 / | \mathbf{r} - \mathbf{r}_i | - \sum_i Z_\alpha e^2 / | \mathbf{r} - \mathbf{r}_\alpha |, \]  

(2.2)

in which \( \mathbf{r} \) and \( \mathbf{r}_i \) are the coordinates of the additional and the \( i \)-th lattice electron respectively and \(-e\) is the electron charge, \( \mathbf{r}_\alpha \) is the equilibrium position of the \( k \)-th ion in the \( l \)-th unit cell, with its charge \( Z_\alpha e \), \( l \) is the abbreviation of the three cell-indices: \( l = (l_1, l_2, l_3) \), \( V_p \) is the interaction of the additional electron and the polarization field induced by the lattice vibration:

\[ V_p = -e \Phi(\mathbf{r}), \]  

(2.3)

where the polarization potential \( \Phi \) is to be calculated by the Poisson equation from the electric polarization \( \mathbf{P}(\mathbf{r}) \):

\[ \Delta \Phi = 4\pi \text{ div } \mathbf{P}(\mathbf{r}). \]  

(2.4)

Finally \( V' \) is the similar interaction of the crystal electrons and the lattice polarization. Now the contributions to the polarization \( \mathbf{P}(\mathbf{r}) \) come mainly from the modes of lattice vibration of longer wave length, and as we concern in the following with the diatomic ionic lattices, we put

\[ \mathbf{P}(\mathbf{r}) = (Ze/\Delta) (\mathbf{u}_1 - \mathbf{u}_2), \]  

(2.5)

the unit cell of volume \( \Delta \) contains two ions of charge \( Ze \) and \(-Ze\), displacements of which are denoted here by \( \mathbf{u}_1 \) and \( \mathbf{u}_2 \) respectively. In (2.5) \( \mathbf{u}_1 - \mathbf{u}_2 \) is assumed to be a continuous function of the position of the unit cell \( l \).

For the harmonic vibrations of the lattice, displacement of each ion can be decomposed into the normal modes of vibration as follows

\[ \mathbf{u}_k = 1/\sqrt{G^3} \sum_j \sum_{\beta} (\mathbf{e}_{\beta j}^{(1)} a_{\beta j} + i q r_j a_{\beta j}^{*}, k = 1, 2, (2.6) \]

where \( G^3 \) is the total number of unit cells, \( \mathbf{e}_{\beta j}^{(1)} \) is to be calculated from the unit vectors of polarization for the normal mode with the propagation vector \( q \) belonging to the \( j \)-th branch of vibration as follows:

- for the optical branch, \( j = 1, 2, 3, \)

\[ \mathbf{e}_{\beta j}^{(1)} = (\sqrt{\mu / M}) e_{\beta j}^{*}, \quad \mathbf{e}_{\beta j}^{(2)} = -(\sqrt{\mu / M}) e_{\beta j}^{*}, \]  

(2.7)

and for the acoustical branch, \( j = 4, 5, 6, \)

\[ \mathbf{e}_{\beta j}^{(3)} = (1/M_1 + M_2) \mathbf{e}_{\beta j}^{*}, \quad k = 1, 2, \]  

(2.7')
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where \( M_1, M_2 \) are the masses of the positive and negative ion respectively and 
\[ \mu = (M_1 M_2 / M_1 + M_2) , \]
\[ a_{qj}^+ \] and \( a_{qj}^- \) are the quantized amplitudes of the normal 
modes of vibration \((q, j)\), of which only the following matrix elements differ 
from zero,
\[
(N_{qj}^+ | a_{qj}^+ | N_{qj}^+ + 1) = \sqrt{\hbar / 2 \omega_q} (N_{qj}^+ + 1), \tag{2.8}
\]
\[
(N_{qj}^- | a_{qj}^- | N_{qj}^- - 1) = \sqrt{\hbar / 2 \omega_q} N_{qj}^-, \tag{2.8'}
\]
where \( N_{qj}^\pm \) is the number of phonons of mode \( q, j \). From (2.3), (2.4), (2.5), 
(2.6) we find
\[
V_s = \frac{Z^2}{\mu} \frac{4 \pi i}{\sqrt{G}} \sum_q \frac{1}{q} \{ a_q^+ \exp iqr - a_q^- \exp -iqr \}, \tag{2.9}
\]
and similarly
\[
V' = \frac{Z^2}{\mu} \frac{4 \pi i}{\sqrt{G}} \sum_i \sum_q \frac{1}{q} \{ a_q^+ \exp iqr_i - a_q^- \exp -iqr_i \}. \tag{2.10}
\]

Contribution to these potential energies comes only from the longitudinal waves 
of the optical mode, the amplitudes of which we now denote simply as \( a_q^+ \) and 
\( a_q^- \).

As well known, the electric polarization of the ionic crystal lattices is induced 
from (1) the polarization of the charge cloud inside each ion and from (2) the 
relative displacements of the positive with respect to the negative ions. As will 
be seen from the following, in the language of the quantum-mechanical perturba­
tion theory, these two mechanisms of the polarization can be explained to come 
from (1) the virtual excitation of the electronic states of the lattice and from (2) 
the virtual emission and reabsorption of phonons. It is noticeable, however, that 
in the higher stages of the perturbation calculations these two modes are mixed 
up and we can no longer separate them perfectly.

To solve the Schrödinger equation (2.1) approximately, we put
\[
\Psi = \Phi(x_1, x_2, \ldots) \chi(Q) \exp \left( -\frac{i}{\hbar} Wt \right) , \tag{2.11}
\]
where \( \phi, \Phi \) are the wave function of the additional electron and crystal electrons 
respectively and \( \chi \) is the wave function of the lattice vibration. We neglect the 
exchange effect of the additional electron with the lattice electrons and \( x_i \) symbo­
lizes the all coordinates of the \( i \)-th lattice electron, \( Q \) means the vibrational 
variables and \( W \) is the total energy. Inserting (2.11) in (2.1) and multiplying 
(2.1) from the left with \( \Phi^* x^* \), \( x^* \phi^* \) and \( \phi^* \Phi^* \) respectively and integrating over 
the respective coordinates, we obtain three Hartree equations for the wave func­
tions \( \phi, \Phi \) and \( \chi \), namely,
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\[
\{-\hbar^2/2md + \{\Phi^* \chi^* V\chi dx dQ - \varepsilon\}\} \phi(\mathbf{r}) = 0, \quad (2.12)
\]
\[
\{H_e + \{\chi^* \phi^* V\chi dx d\mathbf{r} - \eta\}\} \Phi = 0, \quad (2.13)
\]
\[
\{H_l + \phi^* \Phi^* V\phi \Phi dx d\mathbf{r} - \zeta\} \chi = 0, \quad (2.14)
\]
in which \(\varepsilon, \eta, \zeta\) are the energy of the additional electron, lattice electrons and the lattice vibration respectively. For the ground state wave function of the lattice electrons \(\Phi_0\) and for the wave function of the \(N\)-th vibrational state \(\chi_N\) we put

\[
\Phi_0 = \Phi_0^{(0)} + \Phi_0^{(1)} + \cdots, \quad (2.15)
\]
and

\[
\chi_N = \chi_N^{(0)} + \chi_N^{(1)} + \cdots,
\]
then by the perturbation calculations we get from (2.13) and (2.14) the following expressions for \(\Phi_0\) and \(\chi_N\),

\[
\Phi_0 = \Phi_0^{(0)} + \{\phi^* \Phi^* \sum_{\alpha} \{ \Phi_0^{(0) *} \chi_0^{(0) *} V \Phi_0^{(0) *} \chi_0^{(0)} dx dQ / (\eta_0^{(0)} - \eta_0^{(0)}) + \cdots \}
\]
\[
\chi_N = \chi_N^{(0)} + \{\phi^* \Phi^* \sum_{\alpha} \{ \chi_0^{(0) *} \Phi_0^{(0) *} V \chi_0^{(0) *} \Phi_0^{(0)} dx dQ / (\zeta_0^{(0)} - \zeta_0^{(0)}) + \cdots \}
\]
Thus substituting (2.16) and (2.16') into \(\Phi\) and \(\chi\) of (2.12) we obtain the equation for \(\phi(\mathbf{r})\):

\[
\{-\hbar^2/2md + U_0 + U_1 + U_1^* - \varepsilon\} \phi(\mathbf{r}) = 0 \quad (2.17)
\]
with

\[
U_0(\mathbf{r}) = \sum_{\alpha} \{ \Phi_0^{(0) *} \chi_0^{(0) *} V \Phi_0^{(0) *} \chi_0^{(0)} dx dQ ,
\]
\[
U_1(\mathbf{r}) = \sum_{\alpha} \{ \Phi_0^{(0) *} \chi_0^{(0) *} V \Phi_0^{(0) *} \chi_0^{(0)} dx dQ
\]
\[+ \sum_{\alpha} \{ \Phi_0^{(0) *} \chi_0^{(0) *} V \Phi_0^{(0) *} \chi_0^{(0)} dx dQ,
\]
where the effective potential \(U_0\) is that for the unpolarized lattice and \(U_1 + U_1^*\) denotes the reaction from the lattice polarization.

§ 3. Calculation of the Polarization Potential.

As is mentioned in § 2, substitution of (2.16) and (2.16') into (2.19) separates the polarization potential \(U_1(\mathbf{r})\) into two parts:

\[
U_1 + U_1^* = \int \phi(\mathbf{r}) \{ U_0(\mathbf{r}, \mathbf{r}) + U_0(\mathbf{r}, \mathbf{r}) \} d\mathbf{r'}, \quad (3.1)
\]
in which \(U_0(\mathbf{r}, \mathbf{r'})\) which comes from virtual phonon emission is expressed as follows,
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\[ U_e(\vec{r}, \vec{r}') = \sum_n (| \Phi_n^{(t)}|^2 dx | \chi_n^{(t)} V_1(\vec{r}) \chi_n^{(t)} dQ) \times \]
\[ \times (| \Phi_n^{(t)}|^2 dx | \chi_n^{(t)} V_1(\vec{r}) \chi_n^{(t)} dQ) / (\zeta_n^{(t)} - \zeta_0^{(t)}) + \text{conj. compl.} \]  

(3.2)

while \( U_e(\vec{r}, \vec{r}') \) which comes from virtual electronic excitation is given by

\[ U_e(\vec{r}, \vec{r}') = \sum_n (| \chi_n^{(t)}|^2 dQ | \Phi_n^{(t)} V_1(\vec{r}) \Phi_n^{(t)} dx) \times \]
\[ \times (| \chi_n^{(t)}|^2 dQ | \Phi_n^{(t)} V_1(\vec{r}) \Phi_n^{(t)} dx) / (\zeta_n^{(t)} - \zeta_n^{(t)}) + \text{conj. compl.} \]  

(3.3)

Substitution of (2.9) reduces (3.2) to the form

\[ \left( \frac{Ze^2}{\Delta} \right)^2 \left( \frac{4\pi}{2\mu} \right)^2 \sum_q \frac{1}{q \omega_q^2} \{ N_q^{(t)} \exp iq. \vec{r} - \vec{r}' - (N_q^{(t)} + 1) \exp -iq. \vec{r} - \vec{r}' \} + \text{conj. compl.} \]

thus the terms with \( N_q^{(t)} \)-factor cancel out and we find

\[ U_e(\vec{r}, \vec{r}') = -\left( \frac{Ze^2}{\Delta} \right)^2 \left( \frac{4\pi}{2\mu} \right)^2 \sum_q \frac{1}{q \omega_q^2} \{ \exp iq. \vec{r} - \vec{r}' + \exp -iq. \vec{r} - \vec{r}' \}. \]  

(3.4)

Making use of the Debye's approximation for the vibration spectrum, we put

\[ \sum_q \cdots = \frac{G^2 A}{(2\pi)^3} \int \frac{1}{q} dq dQ, \quad q = 2\pi (3/4\pi A)^{1/3}, \quad dQ = \text{solid angle element} \]

and further we neglect the change of optical mode-frequency with the wave length; putting \( \omega_\infty = \omega_0 \) (Reststrahlenfreqenz), we get

\[ U_e(\vec{r}, \vec{r}') = -\frac{4\pi Ze^2}{\mu \omega_0^3} \frac{e^2}{| \vec{r} - \vec{r}' |} \left( \frac{2}{\pi} \right)^{1/2} \sin \frac{\vec{r} - \vec{r}'}{| \vec{r} - \vec{r}' |} d\vec{r}'. \]  

(3.5)

On the other hand, (3.3) can be simply transformed to

\[ U_e(\vec{r}, \vec{r}') = \sum_n (| \Phi_n^{(t)}|^2 \sum_q | \vec{r} - \vec{r}_t | | \Phi_n^{(t)} dx) \left( | \sqrt{\sum_q} | \vec{r} - \vec{r}_t | | \Phi_n^{(t)} dx) / (\zeta_n^{(t)} - \zeta_n^{(t)}) \right) \]
\[ + \text{conj. compl.} \]  

(3.6)

Before getting into further reduction of (3.6) we notice that from (3.1), (3.5), (3.6) it is shown that the lattice polarization becomes the more prominent as the modulation of the electronic wave function \( \phi(\vec{r}) \) from the plane wave form becomes more and more stronger, until finally our perturbation calculation becomes meaningless for sufficiently large polarization. We should like to remark further that \( U_e(\vec{r}, \vec{r}') \) behaves for \( | \vec{r} - \vec{r}' | \gg \text{lattice constant} \) as \( | \vec{r} - \vec{r}' |^{-1} \) and becomes constant for \( | \vec{r} - \vec{r}' | \ll \text{lattice constant} \) (Fig. 1), but we must remind that in our treatment, the detailed behaviour of the potential inside the unit cell has been
neglected from the beginning (cf. (2.5)) and thus the constant value must be interpreted as the average value of $U_e(\mathbf{r}, \mathbf{r}')$ in the unit cell.

\[ \phi_s = \frac{1}{\sqrt{G^*}} \sum_i S_i \phi_i(\mathbf{r}-\mathbf{r}_i^L) \exp i \mathbf{k} \cdot \mathbf{r}_i^L, \tag{3.7} \]

where $\phi_s$ is an ionic orbital, $\mathbf{k}$ is the propagation vector and $S_i$ means summation with respect to the cell-index $i$. Neglecting the overlappings of the different ionic orbitals, and assuming that the most prominent contributions come from the ionic dipole transitions, we get after some simple reductions

\[ U_e(\mathbf{r}, \mathbf{r}') = \frac{(4\pi)^3}{G^* \xi^2} \sum_k \sum_{k'} \exp i(\mathbf{k} - \mathbf{k'} \cdot \mathbf{r} - \mathbf{r}')/|\mathbf{k} - \mathbf{k'}|^2 \times \]

\[ \times 2^d \sum_s \sum_{s'} \left| \phi_s(\mathbf{r}) \phi_{s'}(\mathbf{r}) d\rho \right|^2 / (\eta_{ks}^{(s)} - \eta_{ks'}^{(s')}), \tag{3.8} \]

where the summations with respect to $s$ and $s'$ are to be carried out on the filled and the empty bands respectively. Disregarding the energy spread of each band we put $\eta_{ks}^{(s)} = \eta_{ks'}^{(s)} \approx \eta_i^{(s)} - \eta_{ks'}^{(s')}$; we can further simplify (3.8) to the following form,

\[ U_e(\mathbf{r}, \mathbf{r}') = 2 \frac{4\pi \xi^3}{d} \left( \sum_{s} \sum_{s'} \left| \phi_s(\mathbf{r}) \phi_{s'}(\mathbf{r}) d\rho \right|^2 / (\eta_{ks}^{(s)} - \eta_{ks'}^{(s')}) \right)^{1/2} / |\mathbf{r} - \mathbf{r}'| \cdot 2/\pi \int_0^{\eta_{ks}^{(s)}} \sin \xi/\xi d\xi, \tag{3.9} \]
with $\tilde{q}=2\pi(3/4\pi d)^{1/4}$.

Remembering that $\rho_i=Z^i\varepsilon^i/\Delta \mu \omega^0$, and $\rho_s=2\varepsilon / \Delta \sum \sum |\phi \phi \phi \phi |^2/(\gamma^0-\gamma^0)$ are the polarizability per unit volume of the lattice, each arising from the ionic displacement and the polarization inside each ion respectively, (2.17) can be written in the form

$$\{-\hbar^2/2m\Delta + U_0(\mathbf{r}) - \int |\phi(\mathbf{r})|^2 F(\mathbf{r}-\mathbf{r'}) d\mathbf{r'} - \epsilon \} \phi(\mathbf{r})=0,$$  \hspace{0.5cm} \text{(2.17')}

with

$$F(\mathbf{r}-\mathbf{r'})=4\pi(\rho_i+\rho_s)2/\pi \cdot \varepsilon^i/|\mathbf{r}-\mathbf{r'}| \int \sin \mathbf{r'} \varepsilon d\mathbf{r'},$$  \hspace{0.5cm} \text{(3.10)}

and $U_0(\mathbf{r})$ is the periodic lattice potential. In the limit of continuous medium we put $\Delta \rightarrow 0$, $\tilde{q} \rightarrow \infty$ and get

$$F(\mathbf{r}-\mathbf{r'})\rightarrow (x-1)\varepsilon^i/|\mathbf{r}-\mathbf{r'}|,$$  \hspace{0.5cm} \text{(3.11)}

if we put $x=1+4\pi(\rho_i+\rho_s)$. $x$ is the dielectric constant of the lattice for low frequencies.

In this limit (2.17) becomes

$$\{-\hbar^2/2m\Delta + U_0(-(x-1)) \varepsilon^i/|\mathbf{r}-\mathbf{r'}| \cdot |\phi(\mathbf{r'})|^2 d\mathbf{r'} - \epsilon \} \phi(\mathbf{r})=0.$$  \hspace{0.5cm} \text{(3.13)}

Similar equation:

$$\{-\hbar^2/2m\Delta + U_0-(1/z_0-1/x) \varepsilon^i/|\mathbf{r}-\mathbf{r'}| \cdot |\phi(\mathbf{r'})|^2 d\mathbf{r'} - \epsilon \} \phi(\mathbf{r})=0,$$  \hspace{0.5cm} \text{(3.14)}

was once proposed by Gurney and Mott in their discussions about the possibility of the self-trapping of an electron in a perfect ionic lattice, which possibility had been suggested by L. Landau. Our result (3.13) differs from (3.14) as to the coefficient of the integral, but our perturbation method presupposes, strictly speaking, that $x-1, z_0-1 \ll 1$ and in this limiting case the discrepancy becomes unnoticeable.

As to the validity of our perturbation method, it should be remarked, that the contribution of the polarization potential to the wave function $\phi(\mathbf{r})$ and the energy $\epsilon$ must be smaller than that from $U_0(\mathbf{r})$. For the above mentioned problem of the electron trapping, such condition will be realized if the binding energy of the trapped electron is much smaller than the distance between the energy bands. Further, the detailed structure of the polarization potential in the unit cell is not taken into account in our theory and this fact introduce negligible errors only for the widely extended wave functions, namely for the excited states of the trapped electron.
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In the preceding paragraphs we have discussed the reaction of lattice polarization for the stationary states of an electron. In this paragraph we shall further concern ourselves with the influence of the lattice polarization to the transition probability. We take two examples;

(A) Excitation of the optical modes of vibration.

The probability of the process in which an electron with momentum $\mathbf{p}$ collides with the lattice and excites a quantum of longitudinal vibration of the optical mode of wave number $\mathbf{q}$ and deflected with the momentum $\mathbf{p}'$ is determined by the following matrix element,

$$
\langle \mathbf{p}', N^*_q + 1 | V_z | \mathbf{p}, N^*_q \rangle + \sum_n' \langle N^*_q + 1, 0 | V' | (N^*_q, n) \rangle \langle \mathbf{p}', n | V_z | \mathbf{p}, o \rangle / [E(\mathbf{p}) - E(\mathbf{p}') + \gamma^{(0)} - \gamma^{(0)}]
$$

$$
+ \sum_n' \langle \mathbf{p}', o | V_z | \mathbf{p}, n \rangle (N^*_q + 1, n | V' | N^*_q, o) / [\gamma^{(0)} - \gamma^{(0)} - \hbar \omega],
$$

where $E(\mathbf{p}) = \mathbf{p}^2 / 2m$, the first term comes from the direct transition and the second and the third terms come through the virtual excitation of the electronic states of the crystal. Taking account of the energy conservation $E(\mathbf{p}) - E(\mathbf{p}') = \hbar \omega$, and the inequality $\hbar \omega \ll \gamma^{(0)} - \gamma^{(0)}$, which condition is generally satisfied for ionic crystals, we can reduce (4.1) to the simpler expression

$$
\langle \mathbf{p}', N^*_q + 1 | V_z | \mathbf{p}, N^*_q \rangle \left[ 1 + \frac{4\pi}{\hbar} \sum_{o} \sum_{n} 2e^2 | r_{\mathbf{p}n}^n \mathbf{p}_n |^2 (\gamma^{(0)} - \gamma^{(0)}) \right],
$$

(4.2)

where the same approximation is used for the electronic eigenfunctions as in § 3. (4.2) shows that the effect of the polarization can be taken into account by the factor $(1 - 4\pi \rho_e)$ which in the case $\rho_e \ll 1$ can be expressed by the dielectric constant $\varepsilon$, namely $(2 - \varepsilon)$.

(B) Excitation of the lattice waves.

Wave functions of the lattice excitation waves are written as

$$
\phi_{\mathbf{k}, n}^{(k)} = 1/\sqrt{G} \sum \phi_{\mathbf{k}}^{(k)} \exp i \mathbf{K} \mathbf{r}_n,
$$

(4.3)

where $\phi_{\mathbf{k}}^{(k)}$ describes the state in which the $k$-th ion in the $l$-th unit cell is excited in its $n$-th state, and $\mathbf{K}$ is the wave vector of the excitation wave. The matrix element for the process, in which the momentum of the additional electron changes from $\mathbf{p}$ to $\mathbf{p}'$ while the $(\mathbf{K}, n)$ excitation wave is excited, comes out to be

$$
\langle \mathbf{p}', \mathbf{K} n | V_z | \mathbf{p}, 0 \rangle + \sum_l (N^*_q, \mathbf{K} n | V^* | N^*_q + 1, 0) \langle \mathbf{p}', N^*_q + 1 | V_z | \mathbf{p}, N^*_q \rangle / [E(\mathbf{p}) - \hbar \omega]
$$

$$
- E(\mathbf{p}') + \hbar \omega] + \sum_l (N^*_q, \mathbf{K} n | V^* | N^*_q - 1, 0) \langle \mathbf{p}', N^*_q - 1 | V_z | \mathbf{p}, N^*_q \rangle / [E(\mathbf{p})]
$$
in which \( \gamma_{kn} \) is the energy of the excitation wave and the first term comes from the direct transition while the other terms come through the virtual excitation of the lattice vibrations. Further reduction of the formula becomes possible by the fact that excitation energies of the excitation waves are generally greater than \( \hbar \omega_0 \). Thus (4.4) is reduced approximately to

\[
(\hat{p}' \hat{K}_n | V_1 | \hat{p}, 0) \{ 1 + (4\pi Z^2 e^2 / \Delta \mu \omega_0^2) \left( \hbar \omega_0 / \gamma_{kn} - \gamma_0 \right) \}. \tag{4.5}
\]

Unlike the case of example (A) the correction factor in (4.5) cannot be simply expressed by the dielectric constant, moreover, here, contrary to the simple phenomenological expectations, the influence of the lattice polarization does not reduce but increase the transition probability. Such difference in the above two examples (A) and (B) is, as can be easily recognized, caused by the difference of the relative magnitudes of the energy change in the transition processes and the virtual excitation energy.

Conclusion.

We have developed a quantum-mechanical perturbation calculation for the reaction of the lattice polarization on the electronic motion and it is found out that the mechanism of the electron trapping in a perfect ionic lattice as proposed by Landau, Gurney and Mott is also expected from our quantum-mechanical viewpoint, though our result has not been in perfect agreement with that of above authors. Further the influence of the lattice polarization on the probability of electronic transitions which take place in an ionic lattice has been examined by two examples and it is pointed out that such influence can not be always accounted for by the simple phenomenological introduction of the empirical dielectric constant.

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References.

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