Path-integral methods in polaron theory

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A systematic presentation of the path-integral variational approach to polaron theory is given. The calculation of the energy, effective mass, radius, mobility, electrical conductivity, magnetic susceptibility, and other characteristics of the polaron is considered, and also the description of its behavior in static magnetic and electric fields for arbitrary values of the electron–phonon coupling constant and the temperature. All calculations are made in the framework of the variational principle for the polaron free energy.

INTRODUCTION

The polaron problem is today taken to refer to a large group of problems relating to the behavior of conduction electrons in polar crystals. After some well-known simplifications,[1,2] the system of an electron and longitudinal optical phonons interacting with it can be described by the Pekar–Fröhlich Hamiltonian

$$\hat{H}=\frac{\hat{\mathbf{p}}^2}{2}+\sum_{\mathbf{k}}\hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}+\sum Q(k)\,(\hat{a}_{\mathbf{k}}+\hat{a}_{-\mathbf{k}})\,e^{i\mathbf{k}\cdot\mathbf{r}}; \qquad (1)$$

$$Q(k)=\left(\frac{2\pi c_v}{\Omega}\right)^{1/2}\frac{e}{k},$$

where $\mathbf{r}$ is the radius vector of the electron, e is its charge, $\hat{\mathbf{p}}=-i\partial/\partial\mathbf{r}$ is the operator of the electron quasimomentum, $\hat{a}_{\mathbf{k}}^{+}$, $\hat{a}_{\mathbf{k}}$ are the operators of creation and annihilation of longitudinal optical phonons with quasimomentum $\mathbf{k}$, which takes values in the first Brillouin zone, Ω is the volume of the system, and $c_0=(\varepsilon_\infty^{-1}-\varepsilon_0^{-1})$ (ε_∞ and ε_0 are the high-frequency and static permittivities of the crystal).[1)]

The strength of the interaction is characterized by the dimensionless parameter $\alpha=e^2c_0/\sqrt{2}$. It is important that in the general case it is not possible to regard α as a small parameter in the polaron problem. In III–V group semiconductors, the interaction may be weak ($\alpha\ll 1$), but in many polar dielectrics and semiconductors of the II–VI group it can be intermediate ($\alpha\sim 1$) and strong ($\alpha\gg 1$) in ionic crystals. Therefore, in the general case it is necessary to give up the assumption that the energy spectrum of the carriers is determined by a weak interaction between them and the field of an ideal lattice and that the only part played by the lattice vibrations is the fact that they lead to comparatively rare transitions between the states of the electrons in the ideal crystal. In polar crystals, the electron–phonon interaction leads to a significant renormalization of the electron spectrum (polaron effect), and also to a comparatively strong scattering of the carriers by optical phonons and to a change in their dispersion law. All this complicates the description of the electrical and optical properties of polar crystals.

Qualitatively speaking, the polaron is an electron that moves together with the lattice polarization which it produces. The polarization is described in terms of additional excitation of longitudinal optical phonons. The main quasiparticle characteristics of a polaron are its self-energy, effective mass, lifetime (associated with scattering of the polaron by optical phonons), and radius. All these characteristics depend on the coupling constant α and the temperature. The task of theory is to calculate these characteristics, to describe the thermodynamics of the electron–phonon system and its kinetic properties and response to external electric and magnetic fields, to study the behavior of a polaron in the Coulomb potential of impurities, and so forth. Intimately related to the polaron problem are such problems as the exciton–phonon interaction in polar crystals (an electron polaron bound by the Coulomb potential to a polaron hole) and the dipolaron problem (two polarons interacting through the polarization of the lattice). Historically, it so happened that strong-coupling polaron theory was initially developed by Landau,[3] Pekar,[1,4] Bogolyubov,[5,6] and Tyablikov,[5,7] and later polarons of weak and intermediate coupling were studied by Fröhlich,[8] Lee, Low and Pines,[9] Gross,[10] and others. The first attempt to construct a theory valid for all values of α was made by Feynman in 1955.[11] The main aim of these studies was to calculate the energy and effective mass of a polaron at zero temperature. The further development of polaron theory was in the direction of consideration of the thermodynamics and dynamics of polarons, their behavior in external fields, and also the creation of new methods for describing the electron–phonon system. Various review papers and conference proceedings have been devoted to discussion of the main achievements of polaron theory.[12–19]

Polaron theory is already a traditional but nevertheless very topical field in the physics of condensed media. The increasing interest evinced for it in recent years is due to the fact that it was only at the end of the sixties and during the seventies that reliable experimental data on the electrical and optical properties of polar crystals began to appear. The most informative experiments are those on cyclotron resonance, optical and magneto-optical measurements, and the study of electrotransport in strong fields and the behavior of hot polarons.[14–17] Studies are made of the dependence of the effective mass on the temperature and strength of an external magnetic field, the possible existence of a phase transition from a free to a localized polaron state,[2)] the observation in the optical spectrum of free polarons of so-called Franck–Condon and relaxed excited states, and the dynamics of polarons in strong electric fields.

The success of the path-integral method in polaron the-

[1)]Here, all quantities are measured in the following units: for masses $m=1$, the effective electron mass in the conduction band; for energy $\hbar\omega_0=1$, where ω_0 is the frequency of the longitudinal optical phonons; for length, $(\hbar/m\omega_0)^{1/2}=1$.

[2)]In this connection, see also Ref. 132.

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ory is due to the following technical features. First, one can exactly eliminate the phonon variables from the problem, which is thus reduced to a single-particle problem described by a nonlocal functional that depends only on the electron paths. Second, after this important simplification of the problem it is easy, using Jensen's inequality, to formulate a variational method of solution, a functional analog of Bogolyubov's variational principle for the free energy of quantum-statistical systems. Third, in the language of functionals it is easy to construct a class of exactly solvable models corresponding to quadratic functionals, and these are used as approximating models for variational calculations. This makes it possible to describe in a unified approach polarons of arbitrary coupling, and, moreover, in a wide range of α values it is possible to obtain an estimate for the ground-state energy that is more accurate than those obtained in the framework of the other existing approximations. By means of this method it is possible to calculate almost all the thermodynamic and dynamic quantities of interest in polaron theory. Of course, there is no *a priori* guarantee that a good approximation for the free energy also approximates well the other polaron quantities (in some cases, this is certainly not so), but, in general, the path-integral variational approach makes it possible to create a unified picture of the behavior of the polaron system in a wide range of values of the parameter α, the temperature, and the frequency and strength of the external fields. We note, however, that these positive features are not the exclusive advantage of the path-integral method. Similar results can be obtained (and in some cases were obtained for the first time) by the technique of elimination of the phonon operators by means of time-ordered products.[20–24] Moreover, the approach of Refs. 21–23 has a number of advantages, particularly with regard to the derivation of rigorously justified results and the proofs of some theorems. Since these questions are fully discussed in Refs. 21–23, we shall not dwell on them here.

The aim of the present review is to give a systematic exposition of polaron theory in the language of path integrals. Although individual results are discussed and compared with the results of other models and with experimental data, the main attention is devoted to methodological questions: how the path-integral representation is obtained for each quantity, how it is calculated in the framework of the variational method, and also the existing difficulties of this approach. In this connection, we discuss in detail some ambiguities that can be found in the literature in the calculation of the effective mass and the polaron electrical conductivity. The exposition is limited to study of free polarons and their behavior in external homogeneous fields, i.e., the bipolaron, polaron–impurity, and exciton–phonon interaction problems are not considered. Application of the path-integral method to these problems can be found in Refs. 25–32 and in the review of Ref. 133.

1. POLARON ENERGY

Definitions

The description of an electron–phonon system in the framework of the Pekar–Fröhlich model reduces formally to study of the behavior of a nonrelativistic particle of momentum $\mathbf{p}$ that interacts with a quantum boson field characterized by momentum $\sum_{\mathbf{k}} \mathbf{k}\hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}$ and energy $\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}$. The operator of the total momentum of the system

$$\hat{\mathbf{P}} = \hat{\mathbf{p}} + \sum_{\mathbf{k}} \mathbf{k}\hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}$$

commutes with the Hamiltonian (1),[6] and, therefore, it is an integral of the motion, forming together with the remaining quantum numbers, the set of which we denote by η, a complete set for determining the energy eigenvalues $E(\eta, \mathbf{P})$ and eigenvectors $|\eta, \mathbf{P}\rangle$ of the Hamiltonian $\hat{H}$. As was shown by Bogolyubov,[6] the mean velocity of the particle in the state $|\eta, \mathbf{P}\rangle$ is determined by the expression

$$\mathbf{v}(\eta, \mathbf{P}) = \langle \eta, \mathbf{P} | \hat{\mathbf{p}} | \eta, \mathbf{P}\rangle = \frac{\partial E(\eta, \mathbf{P})}{\partial \mathbf{P}}. \tag{2}$$

The electron coordinates can be eliminated from the Hamiltonian by means of a Bogolyubov canonical transformation[6]:

$$\hat{b}_{\mathbf{k}} = \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}; \quad \hat{b}_{\mathbf{k}}^{+} = \hat{a}_{\mathbf{k}}^{+} e^{-i\mathbf{k}\cdot\mathbf{r}}; \quad \hat{\mathbf{P}} = \hat{\mathbf{p}} + \sum_{\mathbf{k}} \mathbf{k}\hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}},$$

after which the Hamiltonian takes the form

$$\hat{H} = \frac{1}{2}\Big[\hat{\mathbf{P}} - \sum_{\mathbf{k}} \mathbf{k}\hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}}\Big]^2 + \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}} Q(k)(\hat{b}_{\mathbf{k}}^{+} + \hat{b}_{\mathbf{k}}). \tag{3}$$

We consider the situation at zero temperature ($T = 0$).

Let $|\eta_0, \mathbf{P}\rangle$ be the state of lowest energy $E(\eta_0, \mathbf{P})$ for a small fixed $\mathbf{P}$. The energy $E(\alpha)$ and the effective mass $m^*(\alpha)$ of the polaron ground state are determined by

$$E(\eta_0, \mathbf{P}) = E(\alpha) + \frac{\mathbf{P}^2}{2m^*(\alpha)} + \ldots \tag{4}$$

or,[6] with allowance for (2),

$$E(\eta_0, \mathbf{P}) = E(\alpha) + \frac{1}{2} m^*(\alpha)\, \mathbf{v}^2 + \ldots \tag{5}$$

We now consider the system in the state of thermodynamic equilibrium at the temperature T. The free energy $\Phi(\alpha, \beta)$ of the system is determined by the expression

$$\Phi(\alpha, \beta) = -\frac{1}{\beta} \ln \mathrm{Tr}\, e^{-\beta\hat{H}},$$

where $\beta = 1/kT$, and k is Boltzmann's constant. The polaron free energy $F(\alpha, \beta)$ is usually determined by subtracting from $\Phi(\alpha, \beta)$ the free energy of the phonon field in the absence of the particle[20,35]:

$$F(\alpha, \beta) = \Phi(\alpha, \beta) - \frac{1}{\beta} \sum_{\mathbf{k}} \ln(1 - e^{-\beta})$$

or

$$F(\alpha, \beta) = -\frac{1}{\beta} \ln \frac{\mathrm{Tr}\, e^{-\beta\hat{H}}}{Z_{\mathrm{ph}}}, \tag{6}$$

where

$$Z_{\mathrm{ph}} = \prod_{\mathbf{k}} \frac{1}{(1 - e^{-\beta})}.$$

The mean energy $U(\alpha, \beta)$ and the energy eigenvalue $E(\alpha, \beta)$ of the polaron can be determined from $F(\alpha, \beta)$ as follows[20,33]:

$$\left.\begin{aligned} U(\alpha, \beta) &= \frac{\partial}{\partial\beta}\beta F(\alpha, \beta); \\ E(\alpha, \beta) &= \frac{\partial}{\partial\beta}\beta F(\alpha, \beta) - \frac{3}{2\beta}. \end{aligned}\right\} \tag{7}$$

In the limit of zero temperature,

$$\lim_{\beta\to\infty} F(\alpha,\ \beta)=\lim_{\beta\to\infty} U(\alpha,\ \beta)=\lim_{\beta\to\infty} E(\alpha,\ \beta)=E(\alpha). \qquad (8)$$

Path-Integral Representation and Variational Method of Calculation

Representations for the ground-state energy $E(\alpha)$ and the free energy $F(\alpha,\beta)$ of a polaron in the form of path integrals were obtained for the first time by Feynman in Ref. 11 and by Osaka in Ref. 33, respectively. There are various ways of deriving such representations. One of them is based on the Feynman–Kac formula,[34,35] which makes it possible to write the matrix elements $\langle \mathbf{r}', Q' \mid \exp(-\beta\hat{H})\mid \mathbf{r}, Q\rangle$ of the statistical operator of the system in the form of an integral with respect to a Wiener measure[36]:

$$\langle \mathbf{r}',\ Q' \mid e^{-\beta\hat{H}} \mid \mathbf{r},\ Q\rangle = \int\limits_{\mathbf{x}(0)=\mathbf{r}}^{\mathbf{x}(\beta)=\mathbf{r}'} D\mathbf{x} \int\limits_{Q(0)=Q}^{Q(\beta)=Q'} DQ \times \exp\left\{-\int\limits_0^\beta d\tau H[\mathbf{x}(\tau),\ Q(\tau)]\right\},$$

where $H[\mathbf{x}(\tau), Q(\tau)]$ is the Hamiltonian of the system:

$$\left.\begin{aligned} H[\mathbf{x},\ Q] &= \frac{1}{2}\dot{\mathbf{x}}^2+\frac{1}{2}\sum_{\mathbf{k}}(\dot{q}_{\mathbf{k}}^2+q_{\mathbf{k}}^2) \\ &\quad +\sum_{\mathbf{k}} V\overline{2}\, Q(k)\, q_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{x}}-\sum_{\mathbf{k}}\frac{1}{2}; \\ Q=\{q_{\mathbf{k}}\};\quad \int\limits_{Q(0)=Q}^{Q(\beta)=Q'} DQ\ldots &= \left\{\prod_{\mathbf{k}}\int\limits_{q_{\mathbf{k}}(0)=q_{\mathbf{k}}}^{q_{\mathbf{k}}(\beta)=q_{\mathbf{k}}'} Dq_{\mathbf{k}}\right\}\ldots \end{aligned}\right\} \qquad (9)$$

From (9), we obtain for the partition function of the system

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = \int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x} \int\limits_{Q(0)=Q(\beta)} DQ \times \exp\left\{-\int\limits_0^\beta d\tau\, H[\mathbf{x}(\tau),\ Q(\tau)]\right\}.$$

The integrals are taken over all closed paths $\mathbf{x}(\tau)$ of the electron and $q_{\mathbf{k}}(\tau)(0\leqslant\tau\leqslant\beta)$ of the oscillators, and also over all the initial points $\mathbf{x}(0)$ and $q_{\mathbf{k}}(0)$. The integration over the paths of the oscillators can be done by means of general expressions (Ref. 35)[3)]

$$\int\limits_{q(0)=q(\beta)} Dq \exp\left\{-\frac{1}{2}\int\limits_0^\beta du\,[\dot{q}^2+W^2q^2+\gamma q]\right\} = \frac{\exp\left\{\frac{1}{16W}\int\limits_0^\beta\int\limits_0^\beta du\, dv\, \gamma(u)\,\gamma(v)\, C_W(u-v)\right\}}{2\,\mathrm{sh}\,\frac{\beta W}{2}},$$

where

$$C_W(x)=\frac{e^{Wx}}{e^{\beta W}-1}+\frac{e^{-Wx}}{1-e^{-\beta W}}.$$

[3)] *Translator's Note.* The Russian notation for the trigonometric, inverse trigonometric, hyperbolic trigonometric functions, etc., is retained here and throughout the article in the displayed equations.

The result has the form

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = Z_{\mathrm{ph}} \int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x}\, e^{-S[\mathbf{x}]},$$

where

$$\left.\begin{aligned} S[\mathbf{x}] &= \frac{1}{2}\int\limits_0^\beta d\tau\,\dot{\mathbf{x}}^2(\tau)+V[\mathbf{x}]; \\ V[\mathbf{x}] &= -\sum_{\mathbf{k}} Q^2(k)\int\limits_0^\beta d\tau\int\limits_0^\tau d\sigma\, C(\tau-\sigma)\, e^{i\mathbf{k}[\mathbf{x}(\tau)-\mathbf{x}(\sigma)]}; \\ C(\tau) &= C_1(\tau) \end{aligned}\right\} \qquad (10)$$

and in accordance with (6) we obtain for the polaron free energy

$$F(\alpha,\ \beta)=-\frac{1}{\beta}\int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x}\, e^{-S[\mathbf{x}]}. \qquad (11)$$

An equivalent expression was obtained for the first time in Ref. 33. The generalization to the case when the phonon frequency depends on the wave vector $\mathbf{k}$ is obtained by replacing $C(\tau-\sigma)$ by $C_{\omega_{\mathbf{k}}}(\tau-\sigma)$, where $\omega_{\mathbf{k}}$ is the phonon dispersion law.

To obtain a representation for the ground-state energy, we must in accordance with (8) consider the limit $\beta\to\infty$. Then the terms proportional to $e^{-\beta}$ do not contribute to (10). The sum over $\mathbf{k}$ in the first Brillouin zone is replaced by an integral over the complete $\mathbf{k}$ space (continuous limit). We obtain finally

$$\left.\begin{aligned} E(\alpha) &= -\lim_{\beta\to\infty}\frac{1}{\beta}\ln\int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x}\, e^{-S_\Phi(\mathbf{x})}; \\ S_\Phi(x) &= \frac{1}{2}\int\limits_0^\beta d\tau\,\dot{\mathbf{x}}^2(\tau)-\frac{\alpha}{2^{3/2}}\int\limits_0^\beta\int\limits_0^\beta d\tau\, d\sigma\frac{e^{-|\tau-\sigma|}}{|\mathbf{x}(\tau)-\mathbf{x}(\sigma)|}. \end{aligned}\right\} \qquad (12)$$

The functional quadratures in (11) and (12) cannot be calculated exactly, and approximate procedures must be developed for their calculation. Very helpful here was the functional analog of Bogolyubov's variational method for the free energy of quantum-statistical systems.[37] For the calculation of $E(\alpha)$ it was formulated in Ref. 11 and was later generalized to the case of finite temperatures in Ref. 33.

Let $S_0(\mathbf{x})$ be a real functional that approximates $S(\mathbf{x})$. Using Jensen's inequality, we can readily show that

$$F(\alpha,\ \beta)\leqslant F_0+\frac{1}{\beta}\langle S(\mathbf{x})-S_0(\mathbf{x})\rangle_{S_0}, \qquad (13)$$

where F_0 is the free energy of the system described by the action functional $S_0(\mathbf{x})$:

$$\left.\begin{aligned} F_0 &= -\frac{1}{\beta}\ln\int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x}\, e^{-S_0(\mathbf{x})}; \\ \langle A[\mathbf{x}]\rangle_{S_0} &= \frac{\int\limits_{\mathbf{x}(0)=\mathbf{x}(\beta)} D(\mathbf{x})\, e^{-S_0(\mathbf{x})}A[\mathbf{x}]}{\int\limits_{x(0)=\mathbf{x}(\beta)} D\mathbf{x}\, e^{-S_0(\mathbf{x})}}. \end{aligned}\right\} \qquad (14)$$

In particular, at zero temperature

$$E(\alpha)\leqslant E_0+\lim_{\beta\to\infty}\frac{1}{\beta}\langle S-S_0\rangle_{S_0}, \qquad (15)$$

where $E_0 = \lim_{\beta\to\infty} F_0$ is the ground-state energy of the system described by the action functional $S_0(\mathbf{x})$.

If we choose for S_0 the action functional of the free particle,

$$S_0 = \frac{1}{2}\int_0^\beta d\tau\, \dot{\mathbf{x}}^2(\tau),$$

then we obtain the result of the second order of perturbation theory,

$$E(\alpha) \leqslant -\alpha,$$

which, thus, is an upper bound for the ground-state energy. If S_0 is chosen in the form

$$S(\mathbf{x}) = \frac{1}{2}\int_0^\beta d\tau\, \dot{\mathbf{x}}^2(\tau) - \lambda\int_0^\beta d\tau\, \frac{1}{|\mathbf{x}(\tau)|},$$

where λ is the variational parameter determined from the condition of a minimum of the right-hand side of the inequality (15), then the best estimate is given by $F(\alpha) \leqslant -0.098\alpha^2 (\alpha \gg 1)$, which is close to the value obtained by Pekar using Ritz's variational method[1]: $E(\alpha) = -0.1088\alpha^2$.

The difficulties in approximating the action functional $S[\mathbf{x}]$ by the functional $S_0[\mathbf{x}]$ corresponding to motion of a particle in the field of a classical potential $V_{\text{cl}}(\mathbf{x})$ are discussed in detail in Ref. 35. It is found that for $\alpha \lesssim 6$ it is not possible by any choice of $V_{\text{cl}}(\mathbf{x})$ to improve the result obtained for $V_{\text{cl}} = 0$. This shows that, except for the case of very strong coupling, classical approximations do not approximate the real physical situation well. On the one hand, it can be seen from the expression (10) that the action $S[\mathbf{x}]$ is translationally invariant, while the potential field, which acts on the electron at the "time" τ, depends not only on its position $\mathbf{x}(\tau)$ but also on its previous position, i.e., it is determined by the propagation with finite velocity of the disturbance produced by it in the past. On the other hand, any classical potential, the potential $V_{\text{cl}}(x)$ of an external source, will confine the electron near the point of minimum of the potential and depend only on the position of the electron at the given time. For this reason, it is to be expected that for very large α, when the perturbation produced by the electron propagates with very high velocity, the approximation of a classical potential will be more realistic.

Variational Functional and Linear Polaron Model

If in the expression (10) for $S[\mathbf{x}]$ we expand $\exp\{i\mathbf{k}[\mathbf{x}(\tau) - \mathbf{x}(\sigma)]\}$ to powers of $\mathbf{k}$ of second order, omit the constant term, and make the substitutions $\sum_{\mathbf{k}} \frac{k^2 Q^2(k)}{3} \to C$, $C(\tau-\sigma) \to C_W(\tau-\sigma)$, we obtain the functional

$$S_0[\mathbf{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\mathbf{x}}^2(\tau) + C\int_0^\beta d\tau \int_0^\tau d\sigma\, C_W(\tau-\sigma)\,|\mathbf{x}(\tau)-\mathbf{x}(\sigma)|^2. \qquad (16)$$

The functional $S_0(\mathbf{x})$ is the action [the analog of $S(\mathbf{x})$ in the Pekar–Fröhlich model] for a system in which the electron is coupled, not to the lattice, but to some other particle of mass M by means of a "spring," i.e., for the model described by the Hamiltonian

$$\hat{H}_{\mathbf{F}} = \frac{\hat{\mathbf{p}}^2}{2} + \frac{\hat{\mathbf{p}}'^2}{2M} + \frac{1}{2}k\,|\mathbf{r}-\mathbf{r}'|^2, \qquad (17)$$

where $W = \sqrt{k/M}$ and $C = MW^3/4$. It can be seen from the expression (16) that $S_0[\mathbf{x}]$ is translationally invariant, and the potential acting on the electron is also determined by the prehistory of its motion, as for the functional $S[\mathbf{x}]$. In addition, all the path integrals that occur in (13) and (15) for S_0 can be calculated explicitly.[11,33] The optimal values of the variational parameters C and W are determined as functions of α and β by the condition of a minimum of the right-hand side of (13).

An action functional of the form $S_0[\mathbf{x}]$ for the electron is also obtained in Bogolyubov's linear model of electron–phonon coupling[21–23,38] determined by the Hamiltonian

$$\left.\begin{aligned}\hat{H}_0 &= \frac{1}{2}\hat{\mathbf{p}}^2 + \frac{1}{2}W^2(\nu^2-1)\,r^2 + \sum_{\mathbf{k}} W\hat{a}_{\mathbf{k}}^+ a_{\mathbf{k}} + \\ &+ \sum_{\mathbf{k}} iQ_0(k)\,(\mathbf{k}\cdot\mathbf{r})\,(\hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}}^+); \\ \nu^2 &= 1 + \frac{2}{3}\sum_k \frac{k^2 Q_0^2(k)}{W^3}.\end{aligned}\right\} \qquad (18)$$

The Hamiltonian $\hat{H}_0$, like the Pekar–Fröhlich Hamiltonian, has the properties of translational invariance. Here, the part of the total momentum, commuting with the Hamiltonian, is played by the operator

$$\hat{\mathbf{P}}_0 = \mathbf{p} - \sum_{\mathbf{k}} \frac{\mathbf{k}}{W} Q_0(k)\,(\hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}}^+).$$

If we denote by $E_0(\eta, \mathbf{P}_0)$ and $|\eta, \mathbf{P}_0\rangle$ the energy eigenvalues and eigenfunctions of $\hat{H}_0$, then for the mean velocity of the particle in the state $|\eta, \mathbf{P}_0\rangle$ we have[38]

$$V(\eta, \mathbf{P}_0) = \langle \eta, \mathbf{P}_0 | \mathbf{p} | \eta, \mathbf{P}_0\rangle = \frac{\partial E_0(\eta, P_0)}{\partial \mathbf{P}_0}. \qquad (19)$$

The electron coordinates can be eliminated from the Hamiltonian by means of the canonical transformation[21]

$$\hat{a}_{\mathbf{k}} = \hat{b}_{\mathbf{k}} - \frac{i(\mathbf{k}\cdot\mathbf{r})\,Q_0(k)}{W}; \quad \hat{a}_{\mathbf{k}}^+ = \hat{b}_{\mathbf{k}}^+ + \frac{i(\mathbf{k}\cdot\mathbf{r})\,Q_0(k)}{W};$$

$$\hat{\mathbf{P}}_0 = \hat{\mathbf{p}} - \sum_{\mathbf{k}} \frac{\mathbf{k}}{W} Q_0(k)\,(\hat{b}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^+).$$

Then the Hamiltonian becomes

$$\hat{H}_0 = \frac{1}{2}\Big[\hat{\mathbf{P}}_0 + \sum_{\mathbf{k}} \frac{\mathbf{k}}{W} Q_0(k)\,(\hat{b}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^+)\Big]^2 + \sum_{\mathbf{k}} W\hat{b}_{\mathbf{k}}^+\hat{b}_{\mathbf{k}}. \qquad (20)$$

It is not difficult to diagonalize $\hat{H}_0$ by canonical transformations of the phonon operators. The result is[38]

$$\hat{H}_0 = \frac{3}{2}W(\nu-1) + \frac{\hat{\mathbf{P}}_0^2}{2\nu^2} + \sum_{\mathbf{k}} W\hat{C}_{\mathbf{k}}^+\hat{C}_{\mathbf{k}} + \sum_{i=1}^{3} W(\nu-1)\,\hat{C}_{\mathbf{k}_i}^+\hat{C}_{\mathbf{k}_i}, \qquad (21)$$

where $\hat{C}_{\mathbf{k}}^{+}$, $\hat{C}_{\mathbf{k}}$ are new phonon creation and annihilation operators. The operator of the electron momentum can be expressed in terms of $\mathbf{P}_0$, $\hat{c}_{\mathbf{k}}^{+}$, $\hat{c}_{\mathbf{k}}$ by the formula

$$\hat{\mathbf{p}} = \hat{\mathbf{P}}_0 - \sqrt{2W(\nu^2-1)} \sum_{i=1}^{3} \frac{\mathbf{k}_i}{k_i} (\hat{c}_{\mathbf{k}_i} + \hat{c}_{\mathbf{k}_i}^{+}). \tag{22}$$

It follows from (19) and (21) that for the linear model the ground-state energy E_0 and the effective mass m_0^* of the polaron are given by

$$E_0 = \frac{3}{2} W(\nu - 1); \quad m_0^* = \nu^2. \tag{23}$$

Note that $m_0^* = 1 + M$ is the total mass of the two-particle Feynman model (17). The free energy of the polaron in the linear model is

$$F_0(\beta) = \frac{3}{2} W(\nu-1) + \frac{3}{2\beta} \ln \frac{2\pi\beta}{\nu^2\Omega^{2/3}} + \frac{3}{\beta} \ln \frac{1-e^{-\beta W\nu}}{1-e^{-\beta W}}. \tag{24}$$

Thus, the linear polaron model is an exactly solvable model of the electron–phonon interaction, manifesting the effects of the renormalization of the ground-state energy, the effective mass, and the phonon frequencies. Therefore, if the values of the parameters ν and W are chosen suitably, the linear model can serve as a good initial approximation for calculating the equilibrium polaron characteristics.

The expression (16) makes it possible to generalize the linear model to the case when the electron interacts with a distribution of oscillators of all possible frequencies. In this case, the action functional has the form[39–42]

$$\left.\begin{aligned} S_0[G, \mathbf{x}] &= \frac{1}{2} \int_0^\beta d\tau\, \dot{\mathbf{x}}^2(\tau) + V_0[G, \mathbf{x}]; \\ V_0[G, \mathbf{x}] &= \int_{-\infty}^{\infty} dW\, G(W) \int_0^\beta d\tau \times \\ &\times \int_0^\tau d\sigma\, e^{-W(\tau-\sigma)} |\mathbf{x}(\tau) - \mathbf{x}(\sigma)|^2, \end{aligned}\right\} \tag{25}$$

where the function $G(W)$ satisfies the condition

$$G(-W) = e^{-\beta W} G(W).$$

In the special case of the functional (16),

$$G(W') = \frac{C}{1-e^{-\beta W'}} [\delta(W'-W) - \delta(W'+W)].$$

The effective polaron mass for the model (25) has the form[38]

$$m_0^*(G) = 1 + 4 \int_{-\infty}^{\infty} dW \frac{G(W)}{W^3}.$$

Use of the Variational Principle

All the path integrals in (13) and (15) can be expressed in terms of the correlation function

$$J_{\mathbf{k}}(\tau - \sigma) = \langle e^{i\mathbf{k}\cdot[\mathbf{x}(\tau) - \mathbf{x}(\sigma)]} \rangle_{S_0}. \tag{26}$$

The explicit form of the integral (26) for the functionals (16) and (25) can be found in Refs. 33 and 41.

In particular, it is possible to calculate $E(\alpha)$ and $F(\alpha, \beta)$ for different values of α and β. For this, it is necessary to find the optimal values of the parameters ν and W as functions of α and β. In the general case, the problem must be solved by numerical methods, but some limiting cases can be treated analytically:

a) for zero temperature and weak coupling[11]

$$\nu = 1 + 2\alpha/27; \quad W = 3; \quad E(\alpha) \leqslant -\alpha - \alpha^2/81; \tag{27}$$

b) for zero temperature and strong coupling[11]

$$\nu = \frac{4\alpha^2}{9\pi} - 2(2\ln 2 + \tilde{C}) + 1; \quad \tilde{C} = 0{,}5772; \quad W = 1; \tag{28}$$
$$E(\alpha) \leqslant -\frac{\alpha^2}{3\pi} - \frac{3}{2}\left(2\ln 2 + \tilde{C} + \frac{1}{2}\right);$$

c) for low temperature ($\beta \gg 1$) and weak coupling[43]

$$\left.\begin{aligned} \nu &= 1 + \frac{2\alpha}{27} + \frac{7}{9}\frac{\alpha}{\beta}; \quad W = 3\left(1 - \frac{15}{4\beta}\right); \\ F(\alpha, \beta) &\leqslant \frac{3}{2\beta} \ln \frac{2\pi\beta}{\Omega^{2/3}} - \alpha\left(1 + \frac{1}{4\beta}\right) - \frac{\alpha^2}{81}\left(1 + \frac{2}{\beta}\right); \end{aligned}\right\} \tag{29}$$

d) for low temperature and strong coupling[43]

$$\left.\begin{aligned} \nu &= \frac{4\alpha^2}{9\pi} - 2(2\ln 2 + \tilde{C}) + 1 + \frac{6}{\beta}; \quad W = 1; \\ F(\alpha, \beta) &\leqslant \frac{3}{2\beta} \ln \frac{2\pi\beta}{\Omega^{2/3}} - \frac{\alpha^2}{3\pi} - \\ &- \frac{3}{2}\left(2\ln 2 + \tilde{C} + \frac{1}{2}\right) + \frac{3}{\beta}\left(1 - \ln \frac{4\alpha^2}{9\pi}\right); \end{aligned}\right\} \tag{30}$$

e) for $\beta \ll 1$ and $\alpha\sqrt{\beta} \ll 1$, $\nu = 1 + 0(\alpha\sqrt{\beta})$, $W = 6.50/\beta$ (Ref. 20)

$$\left.\begin{aligned} F(\alpha, \beta) &\leqslant \frac{3}{2\beta} \ln \frac{2\pi\beta}{\Omega^{2/3}} - \alpha\left(\frac{\pi}{\beta}\right)^{1/2}\left(1 + \frac{\beta^2}{48}\right) - \\ &- \frac{\pi\alpha^2}{12}(0{,}0804 - 0{,}00132\beta^2); \\ E(\alpha, \beta) &= -\frac{\alpha}{2}\left(\frac{\pi}{\beta}\right)^{1/2}(1 + 0{,}024\alpha\beta^{1/2}). \end{aligned}\right\} \tag{31}$$

Using a computer, Schultz[44] showed that the values of $E(\alpha)$ for $3 \leqslant \alpha \leqslant 11$ are lower (and therefore better) than all the estimates previously obtained. All the numerical results and asymptotic expressions (for $\alpha \to 0$ and $\alpha \to \infty$) for $E(\alpha)$ are compared in Ref. 45.

The corrections to the results of Ref. 11 with allowance for the terms of second order in $S - S_0$ in the expansion

$$F(\alpha, \beta) = F_0 + \frac{1}{\beta}\langle S - S_0\rangle_{S_0} - \frac{1}{2\beta}[\langle (S-S_0)^2\rangle_{S_0} - \langle S - S_0\rangle_{S_0}^2] + \ldots \tag{32}$$

were obtained in Refs. 45 and 46. The result of Ref. 46 agrees with the exact result of fourth-order perturbation theory.[47,48] For strong coupling, the results of Refs. 45 and 46 are closer to the best estimate of adiabatic perturbation theory of Pekar, Bogolyubov, and Tyablikov[1,5–7]:

$$E(\alpha) = -0{,}1085\alpha^2 - 3/2.$$

The asymptotic behavior of $E(\alpha, \beta)$ for $\beta \gg 1$ and $\alpha \ll 1$ has the form[43]

$$E(\alpha, \beta) = -\alpha + \frac{9}{32}\frac{\alpha}{\beta^2}. \tag{33}$$

In Refs. 49 and 50, Feynman's model was generalized to the case when the action functional has the form

$$S_0[\mathbf{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\mathbf{x}}^2(\tau) + \frac{1}{2}\sum_{n=1}^{2} C_n \int_0^\beta \int_0^\beta d\tau\, d\sigma\, e^{-W_n|\tau-\sigma|}\,|\mathbf{x}(\tau)-\mathbf{x}(\sigma)|^2,$$

where C_1, C_2, W_1, W_2 are variational parameters. Calculation of the ground-state energy by the variational method leads to a small improvement of Feynman's estimate, by 0.08% for $\alpha = 3$ and by 0.15% for $\alpha = 5$. In the weak-coupling limit the result of the calculations is $E(\alpha) \leqslant -\alpha - 0.012583\alpha^2$. Another generalization of Feynman's model was proposed in Ref. 45. It was analyzed in detail in Ref. 132. The discontinuities in the derivative $E'(\alpha)$ at $\alpha \simeq 5.8$ and large values of α (see Ref. 132) are interpreted as a phase transition of the polaron from an unlocalized state ($\alpha < 5.8$) to a localized state ($\alpha > 5.8$), and the critical value $\alpha_c = 5.8$ is associated with the radius of convergence of the perturbation series, which according to the arguments of Refs. 51 and 52 must be finite. These discontinuities were also obtained in Refs. 51–60 and 132, but with values $\alpha_c \sim 6$–50. In our view, the question of phase transitions with respect to α posed in Ref. 61 has not yet been solved.

The effect of the finiteness of the Brillouin zone was considered in Ref. 44. In this study, the first Brillouin zone was replaced by a sphere of radius $k_0 = 2\pi/a$, where a is the lattice constant. The continuous limit corresponds to $k_0 \to \infty$. Schultz estimated the relative shift of $E(\alpha)$ for $\alpha = 5$ and $0 \leqslant a \leqslant R_0/0.9$, where $R_0 = (2W\nu)^{-\frac{1}{2}}$ is the polaron radius in Feynman's model. It was shown that the relative shift is less than or of the order of 11%. It is assumed that at very high temperatures the polaron self-energy must vanish and its effective mass must become the mass of a conduction electron. This is due to the fact that the thermal motion breaks up the ion polarization that the electron produces around itself. However, such a picture is not realized in the calculations given above. In accordance with (31), $E(\alpha, \beta) \to -\infty$ as $\beta \to 0$. In Refs. 62 and 63, this situation was explained by the fact that the definitions (6) and (7) do not take into account the changes in the energy of the phonon subsystem due to the renormalization of the phonon frequencies by the electron–phonon interaction. According to this point of view, part of the free energy $F(\alpha, \beta)$ and the self-energy $E(\alpha, \beta)$ is to be ascribed, not to the polaron, but to the phonons, whose frequencies change by an amount $\delta\omega(\mathbf{k})$ proportional to Ω^{-1}. Of course, the procedure of "dividing" the interaction energy between the polaron and the phonons is to a large degree arbitrary, but however we do it, it does not vanish in the limit $\beta \to 0$ in the framework of the existing approximate methods of calculating the energy for the Pekar–Fröhlich model. When one considers one electron interacting with a macroscopic subsystem, a more natural picture is one in which the properties of the macroscopic subsystem are not modified by its interaction with the electron, and the effect of the interaction leads only to a change in the energies of the electron states and to transitions between them.

Note that c_0 must vanish at very high temperatures. This must lead to an "undressing" of the polaron that, if α is regarded as constant, is evidently not contained in the Pekar–Fröhlich model.

Allowance for the finiteness of the Brillouin zone at high temperatures has the consequence that the results (31) are valid under the conditions $\beta \ll 1$, $\alpha\sqrt{\beta} \ll 1$, $\beta k_0^2/2 \gg 1$.

If we let β tend to zero for fixed k_0, we obtain

$$E(\alpha, \beta) = \frac{2\alpha}{\pi}\left(\frac{k_0^2}{2}\right)^{1/2} (\beta k_0^2/2 \to 0).$$

This corresponds to the classical value of the polaron energy determined by the minimum of the functional $S[\mathbf{x}]$:

$$\delta S[\mathbf{x}] = 0;\ \mathbf{x}(0) = \mathbf{x}(\beta),$$

the solution of which is $\mathbf{x}(\tau) = 0$.

2. THE RADIUS OF A POLARON AND THE NUMBER OF EXCITED PHONONS

Definition of the Radius of a Polaron. The Path-Integral Representation

In the framework of the Pekar–Fröhlich model, the electron–phonon interaction is regarded as the interaction between an electron and a polarizable continuum. Let $\hat{\mathbf{P}}(\mathbf{r})$ be the operator of the polarization of the longitudinal optical phonons. Then

$$\hat{\mathbf{H}}_{\text{int}} = e\int_\Omega d^3\mathbf{r}'\, \frac{\nabla'\cdot\hat{\mathbf{P}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \tag{34}$$

where the operator of the density $\hat{\rho}(\mathbf{r}) = -\nabla\cdot\hat{\mathbf{P}}(\mathbf{r})$ of the polarization charge is given by

$$\hat{\rho}(\mathbf{r}) = -\frac{1}{2}\sum_{\mathbf{k}}\left(\frac{c_0}{\pi\Omega}\right)^{1/2} k\hat{q}_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}};\ \hat{q}_{\mathbf{k}} = \sqrt{\frac{1}{2}}\,(\hat{a}_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}). \tag{35}$$

It is well known that this will be a good approximation if the main contribution to the interaction energy is made by regions of the crystal at large distances from the electron. The polaron radius is a parameter that makes it possible to establish a quantitative criterion of applicability of such a description (the polaron radius must be much greater than the lattice constant).

Let $\rho(\mathbf{r})$ be the mean density of the polarization charge. The potential energy of the interaction of an electron with this charge distribution is

$$V = e\int_\Omega d^3\mathbf{r}\, \frac{\rho(\mathbf{r})}{|\mathbf{r}|}, \tag{36}$$

and the total charge of the distribution is $q^* = \int_\Omega d^3\mathbf{r}\rho(\mathbf{r})$. The radius of the polaron can be nominally defined as the distance R that must separate the electron from the point charge q^* if the potential energy of their interaction is to be V. It follows that

$$\frac{1}{R(\alpha, \beta)} = \frac{\int_\Omega d^3\mathbf{r}\, \frac{\rho(\mathbf{r})}{|\mathbf{r}|}}{\int_\Omega d^3\mathbf{r}\rho(\mathbf{r})}. \tag{37}$$

For the system described by the statistical operator

$\exp(-\beta\hat{H})$, the density $\rho(\mathbf{r})$ is by definition

$$\rho(\mathbf{r}) = \frac{\int dQ \langle Q | \rho(\mathbf{r}) | Q\rangle \langle 0, Q | e^{-\beta\hat{H}} | 0, Q\rangle}{\int dQ \langle 0, Q | e^{-\beta\hat{H}} | 0, Q\rangle},$$

where the statistical operator is given by the expression (9). After integration over the phonon paths, we arrive at the result[64]

$$\left.\begin{aligned} &\rho(\mathbf{r}) = \frac{ec_0}{\Omega}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \int_0^{\beta/2} d\tau C(\tau) \langle e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle_S;\\ &q^* = ec_0;\\ &\frac{1}{R(\alpha,\beta)} = \frac{4\pi}{\Omega}\sum_{\mathbf{k}}\frac{1}{k^2}\int_0^{\beta/2} d\tau C(\tau)\langle e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle_S, \end{aligned}\right\} \quad (38)$$

where $C(\tau)$ and $\langle e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle_S$ are defined in Sec. 1. Note that if no allowance is made for the temperature dependence of the parameter c_0, the total charge q^* surrounding the electron is constant

Polaron Radius in the Linear Model

In the framework of the linear model (18), the interaction between the electron and the phonons is equivalent to interaction with a fictitious particle of mass $M = \nu^2 - 1$ bound to the electron by a spring. Therefore, for the polaron radius R_0 one must here take the distance at which one must fix the fictitious particle from the electron to make its potential energy with the electron equal to the mean value of the potential energy, i.e.,

$$R_0^2 = \frac{\mathrm{Tr}(\mathbf{r}-\mathbf{r}')^2 e^{-\beta\hat{H}_\Phi}}{\mathrm{Tr}\, e^{-\beta\hat{H}_\Phi}}, \quad (39)$$

whence[38]

$$R_0^2 = \frac{3}{2W\nu}\operatorname{cth}\frac{\beta W\nu}{2}. \quad (40)$$

In the limit $\beta\to\infty$, $R_0^2 \to \frac{3}{2W\nu}$ this result was obtained for the first time in Ref. 44. At zero temperature and in the case of weak coupling, we obtain, taking into account (27),

$$R_0 = \frac{1}{\sqrt{2}}\left(1 - \frac{\alpha}{27}\right), \quad \alpha \ll 1,$$

while for $\alpha \gg 1$ it follows from (29) that

$$R_0 = \frac{3}{2\alpha}\sqrt{\frac{3\pi}{2}}, \quad \alpha \gg 1.$$

The value of $R_0 = \sqrt{3/2W\nu}$ was also compared with the lattice constant of various ionic crystals in Ref. 44.

Calculation of the Polaron Radius

To calculate $R(\alpha,\beta)$ and $\rho(r)$ in the framework of the variational method, it is necessary to replace $\langle e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle_S$ by $\langle e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle_{S0}$ in the expression (38). In the path-integral approximation, we obtain[43]

$$\left.\begin{aligned} &\frac{1}{R(\alpha,\beta)} = \nu\sqrt{\frac{2}{\pi}}\int_0^{\beta/2} d\tau C(\tau) f^{-1/2}(\tau);\\ &\rho(r) = \frac{ec_0\nu^3}{(2\pi)^{3/2}}\int_0^{\beta/2} d\tau C(\tau) f^{-3/2}(\tau)\exp\left[-\frac{r^2\nu^2}{2f(\tau)}\right]. \end{aligned}\right\} \quad (41)$$

The values of ν and W in (41) can be determined from the condition of a minimum of the free energy. Thus, it is possible to study the dependence of the polaron radius and charge density on the temperature and the coupling constant. Let us consider some limiting cases[43]:

a) $\beta = \infty$; $\alpha \ll 1$; $R(\alpha) = \sqrt{\frac{1}{2}}\left(1 - \frac{2\alpha}{81}\right)$;

as $\alpha\to 0$ $R(\alpha)\to R(0) = \frac{1}{\sqrt{2}}$ and

$$\rho(r) \to \frac{ec_0}{2\pi r}\exp\left\{-\frac{r}{R(0)}\right\};$$

b) $\beta = \infty$; $\alpha \gg 1$; $R(\alpha) = \frac{3\pi}{2\alpha}\sqrt{\frac{1}{2}}$;

c) $\alpha \ll 1$; $\beta \gg 1$; $R(\alpha,\beta) = \sqrt{\frac{1}{2}}\left(1 - \frac{2\alpha}{81} - \frac{1}{4\beta} - \frac{2\alpha}{9\beta}\right)$;

d) $\beta \ll 1$; $\alpha\sqrt{\beta} \ll 1$;

$R(\alpha,\beta) = \sqrt{\beta/2\pi}$, if $\frac{\beta k_0^2}{2} \gg 1$, $k_0\to\infty$;

$R(\alpha,\beta) = \frac{\pi}{2k_0} = \frac{a}{4}$, it $\beta\to 0$, $\frac{\beta k_0^2}{2}\to 0$.

It is evident from these expressions that the polaron radius decreases with increasing value of the coupling parameter α and the temperature and that at very high temperatures the condition $R > a$ is not satisfied. The behavior of $R(\alpha,\beta)$ for $\beta \ll 1$ indicates that at high temperatures the phonon modes with large wave vector play an important part in the electron–phonon interaction.

We now consider the calculation of the number of phonons excited by the interaction and their momentum distribution. In the absence of the electron–phonon interaction, the number of phonons with quasimomentum $\mathbf{k}$ is determined by the Bose–Einstein distribution:

$$N_{\mathbf{k}}^0 = \frac{1}{e^\beta - 1}.$$

The interaction of the electron with the lattice polarization leads to an additional excitation of optical phonons. We have

$$N_{\mathbf{k}} \equiv \langle \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}\rangle = N_{\mathbf{k}}^0 + \delta N_{\mathbf{k}}; \quad \langle \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}\rangle = \frac{\mathrm{Tr}\,\hat{a}_{\mathbf{k}}^+\hat{a}_{\mathbf{k}} e^{-\beta\hat{H}}}{\mathrm{Tr}\, e^{-\beta\hat{H}}}. \quad (42)$$

To find $N_{\mathbf{k}}$, we consider the somewhat more general Hamiltonian

$$\hat{H}_1 = \frac{\hat{\mathbf{p}}^2}{2} + \sum_{\mathbf{k}}\omega(\mathbf{k})\hat{a}_{\mathbf{k}}^+\hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} Q(k)(\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^+)e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (43)$$

Using the Feynman–Hellman theorem, we can write

$$N_{\mathbf{k}} = \left\langle \frac{\delta\hat{H}_1}{\delta\omega(\mathbf{k})}\right\rangle_{\omega(\mathbf{k})=1} = \left.\frac{\delta\Phi_1}{\delta\omega(\mathbf{k})}\right|_{\omega(\mathbf{k})=1}, \quad (44)$$

where $\Phi_1 = -\frac{1}{\beta}\ln\mathrm{Tr}\, e^{-\beta\hat{H}_1}$ is given in accordance with (6), (10), and (11) by

$$\Phi_1 = \frac{1}{\beta}\sum_{\mathbf{k}} \ln \frac{1}{1-e^{-\beta\omega(\mathbf{k})}} - \frac{1}{\beta}\ln \int_{\mathbf{x}(0)=\mathbf{x}(\beta)} D\mathbf{x} e^{-S_1[\mathbf{x}]}, \quad (45)$$

where $S_1[\mathbf{x}]$ is obtained from $S[\mathbf{x}]$ by replacing $C(\tau)$ by $C_{\omega(\mathbf{k})}(\tau)$. Differentiating Φ_1 with respect to $\omega(\mathbf{k})$, we obtain

$$\delta N_{\mathbf{k}} = Q^2(k)\int_0^{\beta/2} d\tau \left[\tau C(\tau) - \frac{1}{2}\frac{\beta \operatorname{sh}\tau}{\operatorname{sh}^2\beta/2}\right]\langle e^{i\mathbf{k}\cdot[\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)]}\rangle_S, \quad (46)$$

where $\tau = |\tau_1 - \tau_2|$. Since $\langle e^{i\mathbf{k}\cdot[\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)]}\rangle_S$ depends only on $|\mathbf{k}|$, for the momentum distribution density of the excited phonons we have

$$n_k = \frac{\Omega}{(2\pi)^3} 4\pi^2 k^2 \delta N_{\mathbf{k}};$$
$$n_k = \frac{\sqrt{2}\alpha}{\pi}\int_0^{\beta/2} d\tau \left[\tau C_*(\tau) - \frac{1}{2}\frac{\beta \operatorname{sh}\tau}{\operatorname{sh}^2\beta/2}\right]\langle e^{i\mathbf{k}\cdot[\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)]}\rangle_S. \quad (47)$$

The total number ΔN of excited phonons is determined by integrating n_k over all values of k.

The expressions (46) and (47) are exact and make it possible to determine n_k as a function of α and β. Note that $n_0 = \sqrt{2}\alpha/\pi$ for α and β. To calculate n_k in Feynman's approximation, it is necessary to replace $\langle e^{i\mathbf{k}\cdot[\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)]}\rangle_s$ by the function $J_{\mathbf{k}}(\tau)$ (26). Making the calculations, we obtain

$$\left.\begin{aligned} n_k &= \frac{\sqrt{2}\alpha}{\pi}\int_0^{\beta/2} d\tau \left[\tau C(\tau) - \frac{1}{2}\frac{\beta \operatorname{sh}\tau}{\operatorname{sh}^2\beta/2}\right] e^{-\frac{k^2}{2v^2} f(\tau)}; \\ N &= \frac{\alpha v}{\sqrt{\pi}}\int_0^{\beta/2} d\tau \left[\tau C(\tau) - \frac{1}{2}\frac{\beta \operatorname{sh}\tau}{\operatorname{sh}^2\beta/2}\right] f^{-1/2}(\tau). \end{aligned}\right\} \quad (48)$$

We consider some limiting cases. At zero temperature,

$$\left.\begin{aligned} n_k &= \frac{\alpha\sqrt{2}}{\pi} e^{-\frac{k^2}{2}\frac{v^2-1}{Wv^3}} \sum_{n=0}^{\infty} \frac{\left(1-\frac{1}{v^2}\right)^n k^{2n}}{(2Wv)^n n!} \frac{1}{\left(1+\frac{k^2}{2v^2}+nWv\right)^2}; \\ n_k &\simeq \frac{\alpha\sqrt{2}}{\pi}\frac{e^{-\mu^2\frac{k^2}{2v^2}}}{\left(1+\frac{k^2}{2v^2}\right)^2}; \\ \Delta N &\simeq \alpha v\left\{\left(\frac{1}{2}-\mu^2\right)[1-erf(\mu)]\, e^{\mu^2} + \frac{\mu}{\sqrt{\pi}}\right\}; \\ \mu &= \frac{v^2-1}{Wv}. \end{aligned}\right\} \quad (49)$$

With increasing α, the numbr of short-wave phonons excited by the interaction increases. In the limit $\alpha \to 0$, ΔN tends to the well-known value $\alpha/2$ and as $\alpha \to \infty$, $\Delta N \to 4\alpha^2/3\pi$. With increasing temperature, the distribution function n_k becomes less steep—more and more short-wave phonons are excited. In the limit $\beta \to 0$, $\alpha\sqrt{\beta} \to 0$, we have $n_k \rightrightarrows \alpha\sqrt{2}/\pi$, $\Delta N \to \alpha\sqrt{2}/k_0/\pi$.

3. EFFECTIVE POLARON MASS

Effective Polaron Mass at Zero Temperature

At zero temperature, when the electron–phonon system is in the state with lowest energy and the number of real phonons is zero, the entire energy and the entire momentum of the system are transported by the polaron. In this case, the effective polaron mass is determined by (4) or (5). Other definitions of the effective mass are possible, namely, in terms of the energy shift of the polaron ground state in a weak magnetic field.[65–69] Such "magnetic" masses are considered in Sec. 4.

To calculate the effective mass of the polaron ground state in the framework of the path-integral variational approach, Feynman[11] proposed that the energy of a polaron moving with velocity $\mathbf{u}$ can be found by generalizing the expression (12) to the case when the integral is taken over all paths $\mathbf{x}(\tau)$ with boundary conditions $\mathbf{x}(0) = 0$, $\mathbf{x}(\beta) = \mathbf{u}\beta$. Thus,

$$\left.\begin{aligned} E(\mathbf{u}) &= E(\alpha) + \frac{1}{2} m_\Phi^* \mathbf{u}^2 + \ldots = \\ &= -\lim_{\beta\to\infty}\frac{1}{\beta}\int_{\mathbf{x}(\beta)=\mathbf{x}(0)+\mathbf{u}\beta} D\mathbf{x} e^{-S_\Phi(\mathbf{x})}. \end{aligned}\right\} \quad (50)$$

Approximate calculation of the path integral in (50) leads to the expression

$$m_F^* = 1 + \frac{\alpha v^3}{3\sqrt{\pi}}\int_0^\infty d\tau e^{-\tau}\tau^2\left[\tau + \frac{v^2-1}{Wv}(1-e^{-Wv\tau})\right]^{-3/2}. \quad (51)$$

When the optimal values of the parameters v and W are substituted in (51), it is possible to estimate the effective mass m_F^* over the complete range of values of the parameter α. In the limiting cases of weak and strong coupling, we obtain

$$m_F^* = 1 + \frac{\alpha}{6} + \frac{2\alpha^2}{81}, \quad \alpha \ll 1;$$
$$m_F^* = \left(\frac{4\alpha^2}{9\pi}\right)^2 - \frac{4\alpha^2}{\pi}(1 + 2\ln 2 + \tilde{C}), \quad \alpha \gg 1.$$

In the leading order in α, these expressions are identical to the results of perturbation theory ($\alpha \ll 1$) and the adiabatic approximation ($\alpha \gg 1$). The coefficient of α^2 in the expression for m_F^* when $\alpha \ll 1$ is 0.024 691. This is close to the exact value of the fourth order of perturbation theory[47,48]: $m^*(\alpha) = 1 + \frac{\alpha}{6} + 0.023676\alpha^2$.

Numerical calculations in accordance with the expression (50) for $\alpha = 3, 5, 7, 9, 11$ were made in Ref. 44. It was shown that m_F^* is somewhat larger than the optimal value of the effective mass of the linear model, $m_0^* = v^2$, but the difference between these quantities is less than 10% and decreases with increasing α.

The determination of the effective mass m_F^* in accordance with (50) is intuitively reasonable and leads to generally accepted results in the well-known limiting cases. However, *a priori* it is not clear whether the mass m_F^* given by (50) and the effective mass m^* determined by the expression (4) are equal (see also Ref. 70). This question is further aggravated by the fact that the direct generalization of the definition (50) to the case of finite temperatures by replacement of the functional $S_F[\mathbf{x}]$ by $S[\mathbf{x}]$ (10) leads to an unphysical result for the effective mass.

In Ref. 20, the effective mass m^* was calculated by means of the asymptotic behavior of the free energy in the

limit $\beta \to \infty$. We note here that the method of determining $m^*(\alpha)$ using the asymptotic behavior does not make it possible to find the temperature dependence of the effective polaron mass.

The effective mass of the polaron ground state ($T = 0$) can also be calculated on the basis of the exact path-integral representation for the lowest energy of the system for a fixed value of the total momentum $E(\eta_0, \mathbf{P})$,[71,72]

$$E(\eta_0, \mathbf{P}) = E(\alpha) + \frac{p^2}{2m^*(\alpha)} + \ldots = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \operatorname*{Tr}_{\mathbf{P}} e^{-\beta\hat{H}}, \tag{52}$$

where the symbol $\operatorname*{Tr}_{\mathbf{P}}$ denotes averaging over the complete set of states of the Hamiltonian (3) for fixed $\mathbf{P}$. The expression (52) can also be written in the form

$$E(\eta_0, \mathbf{P}) = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \int \frac{d^3\mathbf{R}}{(2\pi)^3} e^{i\mathbf{P}\cdot\mathbf{R}} \operatorname{Tr} \{e^{-\beta\hat{H} - i\mathbf{R}\cdot\hat{\mathbf{P}}}\} \tag{53}$$

and leads to the following path-integral representation for $E(\eta_0, \mathbf{P})$:

$$E(\eta_0, \mathbf{P}) = E(\alpha) + \frac{\mathbf{P}^2}{2m^*(\alpha)} + \ldots$$
$$= -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \int \frac{d^3\mathbf{R}}{(2\pi)^3} e^{i\mathbf{R}\cdot\mathbf{P}} \int_{x(\beta)=x(0)+\mathbf{R}} Dx e^{-S\mathbf{F}[x]}. \tag{54}$$

An equivalent expression for $E(\eta_0, \mathbf{P})$ was obtained for the first time in Ref. 71. Calculation in accordance with (54) in the framework of Feynman's variational method leads to the expression (51) for the effective mass $m^*(\alpha)$.[71] Note, however, that the determination of the effective polaron mass through expansion of its energy in powers of the total momentum $\mathbf{P}$ does not admit, in our opinion, direct generalization to the case of finite temperatures. For $T \neq 0$, this expansion strictly speaking does not have a meaning. For $T \neq 0$, a definite fraction of the total momentum of the system is transported by real phonons, and it is impossible to identify $\mathbf{P}$ with the polaron momentum.

In Refs. 49 and 50, the Feynman effective mass (50) was calculated by means of the proposed or generalized variational functional. The result differs from (51) by about 0.4% for $\alpha = 3$ and by 1% for $\alpha = 5$. As was shown in Ref. 44, allowance for the finiteness of the Brillouin zone for $\alpha = 5$ and $0 \leqslant a \leqslant R_0/0.9$ leads to a change in the effective mass m_F^* by $\sim 4\%$ and increases the difference between m_F^* and m_0^*.

Effective Polaron Mass at Finite Temperatures

The temperature dependence of the effective polaron mass was studied in Refs. 33, 43, 62, 64, and 73–80. As we have already said, the definitions (50), (51), and (54) do not admit direct generalization to the case of finite temperatures, and the very question of the definition of the effective polaron mass at a nonzero temperature is rather contentious. This is due, of course, to the fact that at $T = 0$ the electron interacts with the lattice "vacuum" (zero-point vibrations). For $T \neq 0$, real phonons are present and care is needed to define the characteristics of the polaron in this situation.[64] The standard approach to the calculation of the energy, effective mass, and lifetime of quasiparticles at finite temperatures in terms of the single-electron Green's function encounters serious difficulties when applied to the polaron problem. On the other hand, the difficulties are associated with taking into account the translational invariance of the system when formulating various approximations.[81] By the Green's function method it has been possible more or less to progress in the calculation in the first order of perturbation theory in α. The expansion parameter is not α, but $\alpha/(1 - e^{-\beta})$, so that the region of applicability of the resulting expressions contracts with increasing temperature.

On the other hand, the temperature dependence of the effective polaron mass is of undoubted physical interest, in particular in connection with the interpretation of cyclotron-resonance experiments in polar crystals.[82–91] Measurements made in CdTe (Ref. 84) and AgBr (Refs. 85 and 86) crystals in weak magnetic fields ($\omega_c \ll 1$, where ω_c is the cyclotron-resonance frequency) show clearly that the cyclotron mass increases with the temperature at low temperatures ($e^{\beta} \gg 1$). It is not entirely clear[85,86,91] whether a purely polaron effect is observed or whether this is a consequence of the presence of impurities. One way or the other, a detailed discussion of the different approaches to the definition and calculation of the effective mass is worthwhile.

The majority of theoretical studies devoted to the calculation of the effective polaron mass at finite temperatures can be put into one of the following groups.

A. The effective polaron mass is estimated in terms of the effective mass of an approximating model [for example, $m_0^* = \nu^2$ in the case of the model (21)] used to calculate various physical quantities (the free energy in Ref. 33 or the electrical-conductivity coefficient in Ref. 75) for optimal values of the parameters of the model. A shortcoming of such an approach is that it is not clear how to calculate the following corrections in order to establish whether the mass of the model is a good approximation to the value of the effective polaron mass.

B. The effective polaron mass is defined through the change in the free energy or the self-energy of the polaron in a weak external field. In Refs. 77 and 78 it was assumed that in the presence of an electric field of strength $\mathbf{E}$ the system is in the Gibbs state of thermodynamic equilibrium described by the statistical operator $\exp\{-\beta(\hat{H} + e\mathbf{E}\cdot\mathbf{r})\}$. This is a rather strong simplification of the polaron problem in an electric field. We note in this connection that investigations of the exact stationary solution of the Boltzmann equation[92] show that in weak fields the momentum distribution function differs strongly from the Maxwellian form. This renders difficult the physical interpretation of the "inertial mass" of the polaron calculated in Refs. 77 and 78. The "magnetic masses" defined in connection with study of the behavior of a polaron in a magnetic field are discussed in Sec. 4.[67,68]

C. The effective polaron mass is defined in terms of the free energy or mean energy of the system in a mixed state for a fixed mean value of the total momentum (Refs. 43, 62, 64, and 73–80). In such an approach, the following question arises: What fraction of the interaction energy or the total momentum of the system at finite temperatures belongs to

the polaron and what fraction belongs to the phonon subsystem? As we have already noted above in connection with the definition of the polaron energy, the answer to this question is to a certain degree arbitrary, and this leads to a certain arbitrariness in the results. Definite expressions for the effective mass at finite temperatures were obtained in Refs. 43, 62, and 73–80. Most of them predict that $M(\alpha,\beta)\to 1$ in the high-temperature limit $\beta\to 0$.[62,73–80] In the case of low temperatures, it follows from the results of Refs. 33, 43, and 76 that $M(\alpha,\beta)$ increases with the temperature at low temperatures, and in accordance with Refs. 62, 73, and 77–80 the effective polaron mass decreases monotonically for $0\leqslant T<\infty$.

To determine the effective polaron mass, it is necessary to know the additional energy that the system acquires when the particle moves with a small but nonzero mean velocity $\mathbf{v}$. Such is the picture observed in a frame of reference S' moving relative to S with velocity $-\mathbf{v}$. In S', the Hamiltonian $\hat{H}'$, the statistical operator $\hat{\rho}'$, the free energy Φ', and the mean value $\mathbf{P}'$ of the total momentum of the system are given by[64]

$$\left.\begin{aligned}&\hat{H}'=\hat{H}-\mathbf{v}\cdot\hat{\mathbf{P}};\quad \hat{\rho}'=\exp(-\beta\hat{H}');\quad \Phi'=-\frac{1}{\beta}\ln \mathrm{Tr}\,\hat{\rho}';\\&\mathbf{P}=\frac{\mathrm{Tr}\,\hat{\mathbf{P}}\hat{\rho}'}{\mathrm{Tr}\,\hat{\rho}'}.\end{aligned}\right\}\tag{55}$$

To find now the polaron free energy F' and the mean value $\mathbf{\Pi}'$ of the polaron momentum, we must, as in (6), subtract from Φ and $\mathbf{P}'$ the contribution of the phonon field in the absence of interaction in the system S'. We have

$$\left.\begin{aligned}&F'(\alpha,\ \beta,\ \mathbf{v})=\Phi'(\alpha,\ \beta,\ \mathbf{v})-\\&-\frac{1}{\beta}\sum_{\mathbf{k}}\ln\frac{1}{1-e^{-\beta\omega'_{\mathbf{k}}}}=-\frac{1}{\beta}\ln\frac{\mathrm{Tr}\,e^{-\beta(\hat{H}-\mathbf{v}\cdot\hat{\mathbf{P}})}}{Z_{\mathrm{ph}}(\mathbf{v})};\\&\mathbf{\Pi}(\alpha,\ \beta,\ \mathbf{v})=\mathbf{P}'-\sum_{\mathbf{k}}\frac{\mathbf{k}}{e^{\beta\omega'_{\mathbf{k}}}-1}=-\frac{\partial}{\partial\mathbf{v}}F'(\alpha,\ \beta,\ \mathbf{v}),\end{aligned}\right\}\tag{56}$$

where $\omega'_k=1-\mathbf{k}\cdot\mathbf{v}$ are the frequencies of the phonons in the system S', shifted by the Doppler effect. It is assumed that $\mathbf{v}$ is sufficiently small for the inequality $\omega'_{\mathbf{k}}>0$ to hold in the first Brillouin zone. The partition function of the phonon field in the system S' has the form

$$Z_{\mathrm{ph}}(\mathbf{v})=\prod_{\mathbf{k}}\frac{1}{1-e^{\beta\omega'_{\mathbf{k}}}}.$$

If we now define the effective polaron mass $M(\alpha,\beta)$ by means of an expansion of $F'(\alpha,\beta,\mathbf{v})$ in powers of $\mathbf{v}$,

$$F'(\alpha,\ \beta,\ \mathbf{v})=F(\alpha,\ \beta)-\frac{1}{2}M(\alpha,\ \beta)\,\mathbf{v}^2-\ldots,\tag{57}$$

where $F(\alpha,\beta)$, the free energy, is defined by Eq. (6), then it follows from (56) that

$$\mathbf{\Pi}'(\alpha,\ \beta,\ \mathbf{v})=M(\alpha,\ \beta)\,\mathbf{v}+\ldots.\tag{58}$$

Thus, a change in the velocity of the particle by a small amount leads to a change in the polaron momentum by the amount $M(\alpha,\beta)\mathbf{v}$. This makes it possible to give a definite physical meaning to the "thermodynamic" mass $M(\alpha,\beta)$. It is to be expected that under the influence of a weak external force that varies slowly in time compared with the characteristic time of establishment of thermodynamic equilibrium in the system the polaron will behave as a quasiparticle of mass $M(\alpha,\beta)$ with a certain lifetime τ (at low temperatures, τ is very large). Such a picture is realized, for example, under the influence of a weak external electromagnetic field, provided $\omega\ll 1$ (see Sec. 6). Using Eqs. (2), (4), (5), (56), and (57), we can readily show that[64]

$$\lim_{\beta\to\infty}M(\alpha,\ \beta)=m^*(\alpha).\tag{59}$$

We note that already in Ref. 6 Bogolyubov emphasized that the effective mass must be defined as the coefficient of v^2 in the expression for the energy. For the linear model (18), the procedure used above leads to the correct value of the effective mass $m_0^*=v^2$. Indeed, it follows from (21), (23), and (24) that

$$F'_0=-\frac{1}{\beta}\ln\frac{\mathrm{Tr}\,e^{-\beta(\hat{H}_0-\mathbf{v}\cdot\hat{\mathbf{P}})}}{\prod_{\mathbf{k}}(1-e^{-\beta W'})^{-1}}=F_0(\beta)-\frac{1}{2}m_0^*\mathbf{v}^2.\tag{60}$$

Representation in the Form of a Path Integral. Variational Method

In accordance with the definition (57), the calculation of the effective mass $M(\alpha,\beta)$ reduces to calculation of $F'(\alpha,\beta,\mathbf{v})$, which is the free energy of a polaron moving with velocity $\mathbf{v}$. Formally, one can introduce an imaginary velocity $\mathbf{v}=i\mathbf{u}$ and consider the quantity

$$\begin{aligned}F(\alpha,\ \beta,\ \mathbf{u})&=F(\alpha,\ \beta)+\frac{1}{2}M(\alpha,\ \beta)\,\mathbf{u}^2+\ldots\\&=-\frac{1}{\beta}\ln\frac{\mathrm{Tr}\,e^{-\beta[\hat{H}-i\mathbf{u}\cdot\mathbf{P}]}}{Z_{\mathrm{cr}}(i\mathbf{u})}.\end{aligned}\tag{61}$$

For the example of $F(\alpha,\beta,\mathbf{u})$ we now illustrate a different method of obtaining path-integral representations for the variables of the electron–phonon system. To this end, we write the Hamiltonian (3) in the form

$$H=\frac{1}{2}\hat{\mathbf{v}}^2+\hat{H}_0+\hat{H}_i,\tag{62}$$

where $\hat{\mathbf{v}}=\mathbf{P}-\Sigma_{\mathbf{k}}\mathbf{k}\hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}}$, $\hat{H}_0=\Sigma_{\mathbf{k}}\hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}}$, $\hat{H}_i=\Sigma_{\mathbf{k}}Q(k)\times(\hat{b}_{\mathbf{k}}+\hat{b}_{\mathbf{k}}^{+})$. Then

$$\mathrm{Tr}\,e^{-\beta(\hat{H}-i\mathbf{u}\cdot\hat{\mathbf{P}})}=\frac{\Omega}{(2\pi)^3}\int d^3\mathbf{P}e^{i\beta\mathbf{u}\cdot\mathbf{P}}\operatorname*{Sp}_{\mathbf{p}}e^{-\beta\hat{H}_0}\hat{\sigma}(\beta),\tag{63}$$

where $\hat{O}(\tau)=e^{\hat{H}_0\tau}Oe-\hat{H}_0\tau$, $\hat{b}_{\mathbf{k}}(\tau)=\hat{b}_{\mathbf{k}}e^{-\tau}$, $\hat{b}_{\mathbf{k}}^{+}(\tau)=\hat{b}_{\mathbf{k}}^{+}e^{\tau}$. By means of the identity

$$\begin{aligned}\hat{\sigma}(\beta)&=T\exp\left\{-\int_0^\beta d\tau\left[\hat{H}_i(\tau)+\frac{1}{2}\hat{\mathbf{v}}^2(\tau)\right]\right\}\\&=\frac{\int D\eta e^{-\frac{1}{2}\int_0^\beta d\tau\eta^2(\tau)}T\exp\left\{-\int_0^\beta d\tau\,[\hat{H}_i(\tau)+i\eta(\tau)\cdot\hat{\mathbf{v}}(\tau)]\right\}}{\int D\eta e^{-\frac{1}{2}\int_0^\beta d\tau\eta^2(\tau)}},\end{aligned}\tag{64}$$

and bearing in mind that $\mathbf{P}$ commutes with $\hat{H}_0$, we obtain

$$\mathrm{Tr}\, e^{-\beta(\hat{H}-i\mathbf{u}\cdot\hat{\mathbf{P}})} = \int D\eta e^{-\frac{1}{2}\int_0^\beta d\tau\eta^2(\tau)} \times\delta\Big[\int_0^\beta d\tau\eta(\tau) - \mathbf{u}\beta\Big] \prod_{\mathbf{k}} W_{\mathbf{k}}(\eta),$$

where

$$W_{\mathbf{k}}(\eta) = \mathrm{Tr}\Big[e^{-\beta\hat{b}_{\mathbf{k}}^{+}\hat{b}_{\mathbf{k}}} T\exp\Big\{-\int_0^\beta d\tau\,[Q(k)\,\hat{b}_{\mathbf{k}}(\tau) + Q(k)\,\hat{b}_{\mathbf{k}}^{+}(\tau) - i\mathbf{k}\cdot\boldsymbol{\eta}\hat{b}_{\mathbf{k}}^{+}(\tau)\,\hat{b}_{\mathbf{k}}(\tau)]\Big\}\Big]. \tag{64a}$$

Using the results of Ref. 93, we can write $W_{\mathbf{k}}(\eta)$ in the form

$$\left.\begin{aligned} W_{\mathbf{k}}(\eta) &= \frac{1}{1-e^{-\beta\lambda_{\mathbf{k}}}}\exp R_{\mathbf{k}}(\eta);\\ \lambda_{\mathbf{k}}(\eta) &= 1 - i\frac{k}{\beta}\int_0^\beta d\tau\eta(\tau), \end{aligned}\right\} \tag{64b}$$

where

$$R_{\mathbf{k}}(\eta) = Q^2(k)\Big\{\int_0^\beta d\tau_1\int_0^{\tau_1} d\tau_2 e^{\tau_2-\tau_1+i\mathbf{k}\cdot\int_{\tau_2}^{\tau_1} d\tau\eta(\tau)} + \int_0^\beta d\tau_1\int_0^\beta d\tau_2 \frac{e^{\tau_1-\tau_2+i\mathbf{k}\cdot\int_{\tau_1}^{\tau_2} d\sigma\eta(\sigma)}}{e^{\beta\lambda_{\mathbf{k}}}-1}\Big\}.$$

Making now the change $\boldsymbol{\eta}(\tau) = \dot{\mathbf{x}}(\tau)$ of the functional variables and taking into account the definition (63), we arrive at the result obtained in Ref. 64:

$$F(\alpha,\ \beta,\ \mathbf{u}) = -\frac{1}{2}\ln\int_{\mathbf{x}(\beta)=\mathbf{x}(0)+\mathbf{u}(\beta)} Dx\exp\{-S[\mathbf{x},\ \mathbf{u}]\}, \tag{65}$$

where $S[\mathbf{x},\mathbf{u}] = \frac{1}{2}\int_0^\beta d\tau\dot{\mathbf{x}}^2(\tau) + V[\mathbf{x},\mathbf{u}]$ and

$$V[\mathbf{x},\ \mathbf{u}] = -\sum_{\mathbf{k}} Q^2(k)\int_0^\beta d\tau_1\int_0^\beta d\tau_2 \Big[\frac{e^{\tau_2-\tau_1}}{1-e^{-\beta(1-i\mathbf{k}\cdot\mathbf{u})}} + \frac{e^{\tau_1-\tau_2}}{e^{\beta(1+i\mathbf{k}\cdot\mathbf{u})}-1}\Big] e^{i\mathbf{k}\cdot[\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)]}. \tag{66}$$

In the limit $\beta\to\infty$, the expressions (65) and (66) lead to Feynman's expression (50), i.e.,

$$\lim_{\beta\to\infty} F(\alpha,\ \beta,\ \mathbf{u}) = E(\mathbf{u}).$$

Then $\lim_{\beta\to\infty} M(\alpha,\beta) = m_{\mathrm{F}}^*$, from which, with allowance for (59), it follows that $m_{\mathrm{F}}^* = m^*$. For the linear model (18), the quantity analogous to $F(\alpha,\beta,\mathbf{u})$ is determined by the expression

$$F_0(\beta,\ \mathbf{u}) = -\frac{1}{\beta}\ln\frac{\mathrm{Tr}\, e^{-\beta(\hat{H}_0-i\mathbf{u}\cdot\hat{\mathbf{P}}_0)}}{\prod_{\mathbf{k}}\left(\frac{1}{1-e^{-\beta W}}\right)} = F_0(\beta) + \frac{1}{2}m_0^*\mathbf{u}^2 \tag{67}$$

and it is not difficult to obtain for it the following path-integral representation[38]:

$$F_0(\beta,\ \mathbf{u}) = -\frac{1}{\beta}\ln\int_{\mathbf{x}(\beta)=\mathbf{x}(0)+\mathbf{u}\beta} Dx e^{-S_0[\mathbf{x},\ \mathbf{u}]}, \tag{68}$$

where

$$\left.\begin{aligned} S_0[\mathbf{x},\ \mathbf{u}] &= \frac{1}{2}\int_0^\beta d\tau\dot{\mathbf{x}}^2(\tau) + V_0[\mathbf{x},\ \mathbf{u}];\\ V_0[\mathbf{x},\ \mathbf{u}] &= \frac{2C}{W^2}\int_0^\beta d\tau_1\int_0^{\tau_1} d\tau_2 C_W(\tau_1-\tau_2)\,\dot{\mathbf{x}}(\tau_1)\,\dot{\mathbf{x}}(\tau_2). \end{aligned}\right\} \tag{69}$$

Integrating by parts in (69), we can write $V_0[\mathbf{x},\mathbf{u}]$ in the form[38]

$$V_0[\mathbf{x},\ \mathbf{u}] = C\sum_{n=0}^{\infty}\int_0^\beta d\tau_1\int_0^{\tau_1} d\tau_2\{e^{-\beta W n - W(\tau_1-\tau_2)} \times|\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)-\mathbf{u}\beta n|^2 + e^{-\beta W(n+1)+W(\tau_1-\tau_2)}|\mathbf{x}(\tau_1)-\mathbf{x}(\tau_2)-\mathbf{u}\beta(n+1)|^2\}.$$

The last expression can be obtained from (66) in the same way that the functional $S_0[\mathbf{x}]$ is obtained from $S[\mathbf{x}]$ in Sec. 1.

Note that the functionals $S[x,\mathbf{u}]$ and $S_0[\mathbf{x},\mathbf{u}]$ are real for real $\mathbf{u}$. It follows that

$$F(\alpha,\ \beta,\ \mathbf{u}) \leqslant F_0(\beta,\ \mathbf{u}) + \frac{1}{\beta}\langle S[\mathbf{x},\ \mathbf{u}] - S_0[\mathbf{x},\ \mathbf{u}]\rangle_{S_0}^{\mathbf{u}}, \tag{70}$$

where

$$\langle A[\mathbf{x},\ \mathbf{u}]\rangle_{S_0}^{\mathbf{u}} \equiv \frac{\int_{\mathbf{x}(\beta)=\mathbf{x}(0)+\mathbf{u}\beta} Dx e^{-S[\mathbf{x},\ \mathbf{u}]}A[\mathbf{x},\ \mathbf{u}]}{\int_{\mathbf{x}(\beta)=\mathbf{x}(0)+\mathbf{u}\beta} Dx e^{-S[\mathbf{x},\ \mathbf{u}]}}.$$

We see that the effective polaron mass is equal to the mass m_0^* of the linear model plus a correction given by the term $\langle S[\mathbf{x},\mathbf{u}] - S_0[\mathbf{x},\mathbf{u}]\rangle_{S_0}^{\mathbf{u}}$. Thus, the result of Ref. 33 here corresponds to the zeroth approximation.

In the case of the model (25), when the electron interacts with a distribution of oscillators of all possible frequencies, the functional $S_0[G,\mathbf{x},\mathbf{u}]$ has the form

$$S_0[G,\ \mathbf{x},\ \mathbf{u}] = \frac{1}{2}\int_0^\beta d\tau\dot{\mathbf{x}}^2(\tau) + V_0[G,\ \mathbf{x},\ \mathbf{u}];$$

$$V_0[G,\ \mathbf{x},\ \mathbf{u}] = 2\int_{-\infty}^{\infty}\frac{dW}{W^2}G(W)\int_0^\beta d\tau_1\int_0^{\tau_1} \times d\tau_2 e^{-W(\tau_1-\tau_2)}\dot{\mathbf{x}}(\tau_1)\,\dot{\mathbf{x}}(\tau_2)$$

and the effective mass of the model is given by[38]

$$m_0^*(G) = 1 + 4\int_{-\infty}^{\infty}\frac{dW}{W^3}G(W).$$

Dependence of the Effective Polaron Mass on the Temperature

The calculation of the path integrals in (70) leads to the expression

$$F(\alpha,\ \beta,\ \mathbf{u}) \leqslant \frac{3}{2\beta}\ln\frac{2\pi\beta}{\Omega^{2/3}} + \frac{1}{2}\mathbf{u}^2$$

$$-\frac{3}{\beta}\sum_{n=1}^{\infty}\left[1-\frac{(i\omega_n)^2}{Z_0(i\omega_n)}+\ln\frac{(i\omega_n)^2}{Z_0(i\omega_n)}\right]$$
$$-\sum_{\mathbf{k}}Q^2(k)\int_0^{\beta/2}d\tau C_{1-i\mathbf{k}\cdot\mathbf{u}}(\tau)\,e^{-\beta\frac{k^2}{2}\Phi(\tau)};$$
$$\Phi(\tau)=-\frac{4}{\beta^2}\sum_{n=1}^{\infty}\frac{1-\cos\omega_n\tau}{Z_0(i\omega_n)}, \qquad (70a)$$
$$Z_0(\omega)=(\omega+i\varepsilon)^2\left\{1+4\int_{-\infty}^{\infty}dW\frac{P}{W}\frac{G(W)}{W^2-(\omega+i\varepsilon)^2}\right\}.$$

For the effective mass $M(\alpha,\beta)$ we then obtain

$$M(\alpha,\beta)=1+\sum_{\mathbf{k}}\frac{k^2Q^2(k)}{3}\int_0^{\beta/2}d\tau e^{-\beta\frac{k^2}{2}\Phi(\tau)}$$
$$\times\left\{\tau^2C(\tau)-\frac{2\beta\tau}{(e^{\beta}-1)(1-e^{-\beta})}\right.$$
$$\left.\times(e^{\tau}-e^{-\tau})+\beta^2\frac{(e^{\beta}+1)(e^{\tau}+e^{-\tau})}{(1-e^{-\beta})(e^{\beta}-1)^2}\right\}. \qquad (71)$$

On the basis of (71), let us consider some limiting cases.

a) The Case of Low Temperatures. For $e^{-\beta}\ll 1$, we obtain in the path-integral approximation[43]

$$M(\alpha,\beta)=1+\frac{\alpha v^3}{3\sqrt{\pi}}\int_0^{\beta/2}d\tau e^{-v\tau}\tau^2$$
$$\times\left[\tau\left(1-\frac{\tau}{\beta}\right)+\frac{v^2-1}{Wv}(1-e^{-Wv\tau})\right]^{-3/2}. \qquad (72)$$

The expression (72) is a generalization of Feynman's result (51) to the case of low temperatures. Taking into account (29) and (30), for very low temperatures we have[43]

$$M(\alpha,\beta)=1+\frac{\alpha}{6}+\frac{3}{8}\frac{\alpha}{\beta}+\frac{2}{81}\alpha^2+0{,}235\frac{\alpha^2}{\beta},$$
$$\alpha<1,\ \beta\gg 1;$$
$$M(\alpha,\beta)=\left(\frac{4\alpha^2}{9\pi}\right)^2-\frac{4\alpha^2}{3\pi}\left(1+2\ln 2+\tilde{C}-\frac{9}{\beta}\right), \qquad (73)$$
$$\alpha\gg 1,\ \beta\gg 1.$$

The expressions (73) show that the effective polaron mass $M(\alpha,\beta)$ increases with the temperature at low temperatures. This dependency is due to the nonparabolicity of the polaron dispersion law $E(\eta_0,\mathbf{P})$.

In Refs. 43, 82, and 94, the relative shift of the effective polaron mass predicted by (73) is compared with the experimental temperature dependence of the cyclotron masses that is observed in polar crystals for $e^{-\beta}\ll 1$ and $\omega_c\ll 1$. In CdTe [$\alpha=0.4$ (Ref. 88); $\hbar\omega_0/k=245$ °K (Ref. 83)], the mass shift in accordance with (73) for a change in the temperature from 4.2 to 60 °K is 4%, while experimentally it was 5%.[84] In AgBr [$\alpha=1.6$ (Ref. 83); $\hbar\omega_0/k=190$ °K (Ref. 83)] a relative mass shift of 5% was observed in the interval from 4.2 to 19.1 °K (Ref. 85), and 2% from 17 to 23 °K.[86] The expression (73) predicts 7 and 2%, respectively. Note that at low temperatures the effective mass is much more sensitive to the temperature than the polaron self-energy, for which the first temperature correction is of order $\alpha\beta^{-2}$ [see Eq. (33)]. Therefore, no shift of the self-energy was observed in optical-absorption experiments in AgBr in the range from 4.2 to 40 °K (the expected shift was about 3 meV,[82] of the order of the experimental error).[95] If one takes into account the experimental errors, the influence of impurities, the finite value of the magnetic field, and the possibility of taking into account terms of higher order in α and β^{-1}, it may be concluded that the expression (73) explains in principle the temperature dependence of the cyclotron polaron mass. Analytic expressions for the effective polaron mass for $\beta\gg 1$ were also obtained in Refs. 67, 73, 74, 77, 79, and 80.

b) The Case of Very High Temperatures. For $\beta\ll 1$, $v\to 1$ and the expression (71) leads to the result

$$M(\alpha,\beta)=1+\frac{16\alpha}{3\pi\beta}\left(\frac{k_0^2}{2}\right)^{1/2}\left[1-{}_1F_1\left(1,\frac{3}{2},-\frac{\beta k_0^2}{8}\right)\right];$$
$$\alpha\sqrt{\beta}\ll 1, \qquad (73a)$$

where ${}_1F_1(a,b,z)$ is the confluent hypergeometric function. As usual, two limiting cases can be considered:

i) $\beta\ll 1$; $\beta\frac{k_0^2}{2}\gg 1$; $M(\alpha,\beta)=1+\frac{16\mu}{3\pi\beta}\left(\frac{k_0^2}{2}\right)^{1/2}$;

ii) $\beta\gg 1$; $\frac{\beta k_0^2}{2}\ll 1$; $M(\alpha,\beta)=1+\frac{8\alpha}{9\pi}\left(\frac{k_0^2}{2}\right)^{3/2}$.

The last expression corresponds to the classical limit. Such an expression for the effective mass is also obtained by calculating $E(\mathbf{u})$ in the classical approximation, i.e., when the minimum of the functional S_F is sought on paths satisfying the conditions

$$E_{cl}(\mathbf{u})=\lim_{\beta\to\infty}\frac{1}{\beta}S[\mathbf{x}_{cl},\mathbf{u}];$$
$$\delta S[x_{cl},\mathbf{u}]=0;\ \mathbf{x}_{cl}(0)=0,\ \mathbf{x}_{cl}(\beta)=\mathbf{u}\beta. \qquad (74)$$

The solution of the last equation has the form $\mathbf{x}_{cl}(\tau)=\mathbf{u}\tau$. Note that in the limit $\beta\to 0$ the effective mass $M(\alpha,\beta)$ tends, not to unity, but to its classical value. Here, the discussion of the "undressing" of the polaron given in Sec. 1 in connection with the high-temperature behavior of the polaron energy is valid. Note also that the dependence of $M(\alpha,\beta)$ on k_0 for $\beta\ll 1$ agrees with an increasing importance of short-wave phonons in this limit, an indication of which is the behavior of the polaron radius and the distribution of the excited phonons at high temperatures. Expressions for the effective polaron mass for $\beta\ll 1$ were also obtained in Refs. 67, 73, 77, 79, and 80.

4. EQUILIBRIUM CHARACTERISTICS OF A POLARON IN A MAGNETIC FIELD

In the presence of a static homogeneous magnetic field of strength $\mathbf{h}$, the electron–phonon system (1) is described by the Hamiltonian

$$\hat{H}=\frac{1}{2}\left(\hat{\mathbf{p}}+\frac{e}{c}\mathbf{A}\right)^2+\sum_{\mathbf{k}}\hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}+\sum_{\mathbf{k}}Q(k)(\hat{a}_{\mathbf{k}}+\hat{a}_{-\mathbf{k}}^{+})e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad (75)$$

where $\mathbf{A}=\frac{1}{2}(\mathbf{h}\times\mathbf{r})$ is some potential.

The path-integral method was used in Refs. 65–69 and 96 to study the behavior of a polaron in a magnetic field. Of greatest interest is the calculation of the polaron susceptibility,[65,67,69] the ground-state energy and the free energy of a

polaron in the magnetic field.[66,68,96] and the magnetic masses determined on their basis.[65–67,69] In Ref. 96, Peeters and Devreese predicted the existence of a phase transition of the first kind from the localized to the free state of the polaron under the influence of a sufficiently strong magnetic field.

The point of departure for these calculations is the path-integral representation for the free energy of the polaron in the magnetic field[65]:

$$\left.\begin{aligned} F(\alpha,\ \beta,\ \omega_c) &= -\frac{1}{\beta}\ln\frac{\mathrm{Tr}\,e^{-\beta\hat{H}}}{Z_{ph}} \\ &= -\frac{1}{\beta}\ln\int\limits_{x(0)=x(\beta)} Dx e^{-S[x,\ \omega_c]}; \\ S[x,\ \omega_c] &= S[x]+\frac{i\omega_c}{2}\int\limits_0^\beta d\tau\,[x_1(\tau)\dot{x}_2(\tau)-\dot{x}_1(\tau)x_2(\tau)]. \end{aligned}\right\} \tag{76}$$

Here, $S(\mathbf{x})$ is determined by the expression (10), $\omega_c = eh/c$, and it is assumed that the magnetic field $\mathbf{h}$ is directed along the z axis. We note immediately that although the free energy $F(\alpha, \beta, \omega_c)$ is a real quantity, the functional $S[\mathbf{x}, \omega_c]$ is complex. Therefore, the proof of the variational principle for the free energy by means of Jensen's inequality does not apply to $F(\alpha, \beta, \omega_c)$. It is clear that the total free energy $-(1/\beta)\ln\mathrm{Tr}\,e^{-\beta\Xi H}$ of the system satisfies Bogolyubov's inequality,[37] but an inequality of the type (13) for $F(\alpha, \beta, \omega_c)$ has not yet been proved.

The static susceptibility $\chi(\alpha, \beta)$ is defined by

$$\chi(\alpha,\ \beta) = -\frac{\partial^2 F(\alpha,\ \beta,\ \omega_c)}{\partial\omega_c^2}\Big|_{\omega_c=0}$$

in conjunction with the use of (76):

$$\begin{aligned} \chi(\alpha,\ \beta) = -\frac{1}{\beta}\int\limits_0^\beta\int d\tau\,d\sigma\,[&\langle x_1(\tau)\dot{x}_2(\tau)x_1(\sigma)\dot{x}_2(\sigma)\rangle_S \\ &-\langle x_1(\tau)\dot{x}_2(\tau)\rangle_S\langle x_1(\sigma)\dot{x}_2(\sigma)\rangle]. \end{aligned} \tag{77}$$

To calculate $\chi(\alpha, \beta)$ in the quadratic approximation, it is necessary in (77) to replace the functional $S[\mathbf{x}]$ by $S_0[\mathbf{x}]$. For a quadratic functional $\langle x_1(\tau)x_2(\tau)\rangle_{S_0} = 0$ and the approximate expression for $\chi(\alpha, \beta)$ is

$$\chi(\alpha,\ \beta) = \frac{1}{\beta}\sum_{n=1}^{\infty}\frac{\omega_n^2}{Z_0^2(i\omega_n)}. \tag{78}$$

For a free particle $Z_0(i\omega_n) = (i\omega_n)^2$, and the expression (78) leads to the well-known result $\chi_{00}(\beta) = (1/24)\beta$. For the linear model, the susceptibility is

$$\begin{aligned} \chi_0(\beta) = \frac{\beta}{24v^4}+\frac{1}{8Wv^5}(v^2-1)(v^2+3)\,\mathrm{cth}\,\frac{\beta Wv}{2} \\ +\frac{\beta(v^2-1)}{16v^2}\,\mathrm{csch}^2\frac{\beta Wv}{2}. \end{aligned} \tag{79}$$

The low-temperature limit of this expression was obtained for the first time in Ref. 65. By analogy with the expressions for the susceptibility of the free particle and the linear model, the magnetic polaron mass was defined in Ref. 65 by means of the expression

$$\frac{1}{m_H^2} = \lim_{\beta\to\infty}\left[\frac{\chi(\alpha,\ \beta)}{\chi_{00}(\beta)}\right] = \lim_{\beta\to\infty}\frac{24\chi(\alpha,\ \beta)}{\beta}. \tag{80}$$

For a polaron, $Z(i\omega_n)$ can be determined from the variational principle for the free energy by Eq. (71). If to solve this equation by successive approximation we use a zeroth approximation, then for $Z_0(i\omega_n)$ in the first approximation we obtain

$$Z_0(i\omega_n) = (i\omega_n)^2 - \frac{2}{3}\frac{\alpha v^3}{\sqrt{\pi}}\int\limits_0^{\beta/2} d\tau C(\tau)(1-\cos\omega_n\tau)f^{-3/2}(\tau).$$

If we now substitute this expression in (78) and then in (80) and bear in mind that the series in (78) converges uniformly, we obtain

$$m_h = m_F^* = m^* = 1+\frac{\alpha v^3}{\sqrt{\pi}}\int\limits_0^\infty \frac{d\tau\tau^2 e^{-\tau}}{\left[\tau+\frac{v^2-1}{Wv}(1-e^{-Wv\tau})\right]^{3/2}} \tag{81}$$

We consider the approximate expression for the free energy of the polaron in the magnetic field:

$$F(\alpha,\ \beta,\ \omega_c) = F_0(\alpha,\ \beta,\ \omega_c)+\frac{1}{\beta}\langle S-S_0\rangle_{S_0}. \tag{82}$$

As an approximating functional $S_0[\mathbf{x}, \omega_c]$ we take with allowance for the symmetry of the problem

$$\begin{aligned} S_0[x,\ \omega_c] = &\frac{1}{2}\int\limits_0^\beta d\tau\dot{x}^2(\tau) \\ &+\frac{i\omega_c}{2}\int\limits_0^\beta d\tau\,[x_1(\tau)\dot{x}_2(\tau)-\dot{x}_1(\tau)x_2(\tau)] \\ &+\sum_{i=1}^{3}\int\limits_{-\infty}^{\infty} dWG_i(W)\int\limits_0^\beta d\tau\int\limits_0^\tau d\sigma e^{-W(\tau-\sigma)}|x_i(\tau)-x_i(\sigma)|^2, \end{aligned} \tag{83}$$

where

$$G_1(W) = G_2(W) = G_\perp(W); \qquad G_3(W) = G_\parallel(W);$$
$$G_i(-W) = G_i(W)e^{-\beta W}.$$

However, it should be noted that it is not clear whether (82) is an upper bound for the true free energy of the polaron when $\omega_c \neq 0$. The expression for the free energy that follows from (82) and (83) has the form

$$\begin{aligned} F(\alpha,\ \beta,\ \omega_c) = &\frac{3}{2\beta}\ln\frac{2\pi\beta}{\Omega^{2/3}} \\ &-\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\frac{\omega_n^4(i\omega_n)^2}{Z_\parallel(i\omega_n)[Z_\perp^2(i\omega_n)+\omega_n^2\omega_c^2]} \\ &-\frac{1}{\beta}\sum_{n=1}^{\infty}\left\{\frac{\omega_n^2+Z_\parallel(i\omega_n)}{Z_\parallel(i\omega_n)}+\frac{2Z_\perp(i\omega_n)[Z_\perp(i\omega_n)+\omega_n^2]}{Z_\perp^2(i\omega_n)+\omega_n^2\omega_c^2}\right\} \\ &-\sum_{\mathbf{k}}Q^2(k)\int\limits_0^{\beta/2} d\tau C(\tau) \\ &\times\exp\left\{-\frac{\beta}{2}[(k_1^2+k_2^2)\Phi_\perp(\tau)+k_3^2\Phi_\parallel(\tau)]\right\}, \end{aligned} \tag{84}$$

where

$$Z_{ii}(i\omega_n) = (i\omega_n)^2\left\{1+4\mathcal{P}\int\limits_{-\infty}^{\infty}\frac{dW}{W}\frac{G_i(W)}{W^2+\omega_n^2}\right\};$$

$$Z_{11}=Z_{22}=Z_\perp;\ Z_{33}=Z_\parallel;\ \Phi_\perp(\tau)=-\frac{2}{\beta^2}\sum_{n=1}^{\infty}(1-\cos\omega_n\tau)$$
$$\times\left[\frac{1}{Z_\perp(i\omega_n)+i\omega_n\omega_c}+\frac{1}{Z_\perp(i\omega_n)-i\omega_n\omega_c}\right];$$
$$\Phi_\parallel(\tau)=-\frac{4}{\beta^2}\sum_{n=1}^{\infty}\frac{1-\cos\omega_n\tau}{Z_\parallel(i\omega_n)}.$$

The expression (84) is identical to the one obtained in Ref. 68, and for

$$G_\perp(W')=G_\parallel(W')=\frac{C}{1-e^{-\beta W}}[\delta(W'-W)-\delta(W'+W)]$$

leads to the result of Ref. 65.

In the case of a weak magnetic field ($\omega_c \ll 1$) it to be expected that the model which leads to the best estimate of the free energy for $\omega_c = 0$ also gives a good approximation for $F(\alpha,\beta,\omega_c)$. In such a case, expansion of (84) to the second order in ω_c leads to the expression[67]

$$F(\alpha,\ \beta,\ \omega_c)=F(\alpha,\ \beta)+\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\left\{1+\frac{\omega_n^2\omega_c^2}{Z_0^2(i\omega_n)}\right\}.$$

For finite β we readily obtain from this the expression (78) for the susceptibility.[67]

The ground-state energy of the polaron in the weak magnetic field has the form

$$E(\alpha,\ \omega_c)=\lim_{\beta\to\infty}F(\alpha,\ \beta,\ \omega_c)=E(\alpha)+\Delta E(\alpha,\ \omega_c),$$

where $\Delta E(\alpha,\omega_c)$ in the given approximation is

$$\Delta E=\lim_{\beta\to\infty}\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\left\{1+\frac{\omega_n^2\omega_c^2}{Z_0(i\omega_n)}\right\}.$$

For a free particle $\Delta E=\omega_c/2$, and for the linear model $\Delta E=\omega_c/2\nu^2$. By analogy, we can also define one more magnetic mass m_Λ, which determines the renormalization of the energy of the first Landau level due to the electron–phonon interaction[66]:

$$\Delta E=\omega_c/2m_\Lambda.$$

So far as we know, a proof that m_Λ is equal by definition to the effective ground-state mass of the polaron has not been published, though on physical grounds one expects them to be equal. In Ref. 67, it is shown that in the quadratic approximation

$$m_\Lambda=m_H=\lim_{\beta\to\infty}\frac{Z_0(i\omega_n)}{(i\omega_n)^2}.$$

Then, with allowance for (81),

$$m_\Lambda=m_H=m_\Gamma^*=m^* \tag{85}$$

The expression (85) shows that systematic calculation in the framework of the quadratic approximation with allowance for the first correction to the one-oscillator Feynman model leads to equality of all these masses.

In Ref. 96, the ground-state energy of a polaron in an arbitrary magnetic field was calculated using a functional of the type (83) with the special choice

$$G_\perp(W)=\frac{C_\perp}{1-e^{-\beta W_\perp}}[\delta(W-W_\perp)-\delta(W+W_\perp)];$$
$$G_\parallel(W)=\frac{C_\parallel}{1-e^{-\beta W_\parallel}}[\delta(W+W_\parallel)-\delta(W+W_\parallel)];$$
$$C_\parallel=\frac{W_\parallel^3(\nu_\parallel^2-1)}{4};\ C_\perp=\frac{W_\perp^3(\nu_\perp^2-1)}{4}. \tag{86}$$

It was assumed by Peeters and Devreese[96] that the expressions they obtained for $E(\alpha,\omega_c)$ give an upper bound for the true energy of the polaron ground state in the magnetic field, and they minimized it numerically with respect to the parameters $W_\parallel$, $\nu_\parallel$, $W_\perp$, $\nu_\perp$ in the region $\alpha>4$ and $\omega_c>2$. They found that for $\omega_c>2.24$ the derivative $\frac{\partial E(\alpha,\omega_c)}{\partial\alpha}$ has a discontinuity at the point $\alpha_c(\omega_c)>4.21$, and for $\omega_c=2.24$ and $\alpha_c=4.21$ the derivative $\frac{\partial E(\alpha\omega_c)}{\partial\alpha}$ is a continuous function but $\frac{\partial^2 E(\alpha,\omega_c)}{\partial\alpha^2}$ diverges. From this it is concluded that for $\omega_c>2.24$, $\alpha>4.21$ the system undergoes a phase transition of the first kind, while the point $\alpha_c=4.21$, $\omega_c=2.24$ corresponds to a phase transition of the second kind. At the points $(\omega_c,\alpha_c(\omega_c))$ the transverse mass $\nu_\perp^2$ of the model exhibits a discontinuity, and this makes it possible to interpret the phase transition as a transition of the polaron from a bound state in which the electron together with the phonon cloud rotates in the plane perpendicular to the magnetic field, to the free state of lower mass in which the phonon cloud does not succeed in following the motion of the polaron. Experimentally, such a phase transition must be clearly reflected in the magneto-optical spectrum of crystals with a sufficiently strong electron–phonon interaction, for example, for polaron holes in CuCl ($\alpha=4.36$) and TeCl ($\alpha=4.2$). Bogolyubov's linear model for a polaron in a magnetic field was investigated in detail in Ref. 135. It was shown that for an isotropic dependence of the parameter of the electron coupling to phonon modes of equal frequency the Hamiltonian can be diagonalized.

5. POLARON MOBILITY

Kinetic-Equation Method

The problem of electrotransport in polar crystals with allowance for the polaron effect has been widely investigated by various authors in the framework of an approach based on the Boltzmann equation. There is a detailed review of all studies up to 1967 in Ref. 13, so that here we shall discuss only the basic features and difficulties of applying the kinetic-equation method to calculate polaron mobility. A systematic exposition of methods of obtaining kinematic equations for dynamical systems interacting with a boson field and their application to the polaron problem are given in Refs. 21 and 22. A generalization of the Boltzmann equation for a polaron to the case of an arbitrary electric field was obtained in Ref. 97. The investigation of exact steady-state solutions of the Boltzmann equation, the difficulties of the Maxwell approximation, and linearization with respect to the electric field are discussed in Refs. 92, 98, and 99.

It is well known that at sufficiently low temperatures ($\beta\gg 1$) and low frequencies of the external field ($\omega\ll 1$) the electrical conductivity in a polar crystal is determined by

"rare" scattering of carriers by acoustic phonons and impurities. One can then proceed from the concept of the existence of a quasiparticle (polaron) with dispersion law $\varepsilon(\mathbf{p})$, its mean free path being large compared with its de Broglie wavelength. As a consequence, the behavior of the carriers is described by the momentum distribution function $W(\mathbf{p}, t)$, which is determined as the solution of the well-known Boltzmann equation with allowance for the quantum-mechanical nature of the dispersion law of the polarons and the probability of their scattering by the acoustic phonons and impurities. Since the scattering by the acoustic phonons is quasielastic, while the impurity scattering is elastic, it is not necessary to know the wave function or dispersion law of the polaron at high velocities. The mobility has the same form as for electrons in homeopolar crystals, and differs only in the replacement of the effective electron mass by the effective polaron mass $m^*(\alpha)$.

With increasing temperature, there is an increase in the contribution of scattering by optical phonons, which becomes dominant when $\beta \sim 1$. The Boltzmann description is satisfactory if the following conditions are satisfied: a) the interaction is sufficiently weak and the cross section in a single-scattering event can be calculated by perturbation theory in the lowest Born approximation; b) the successive scattering events (absorption and emission of optical phonons) are sufficiently well separated in time, so that the quantum-mechanical interference between them can be ignored. The corresponding Boltzmann equation has the form

$$\frac{\partial W(\mathbf{p}, t)}{\partial t} + e\mathbf{E}(t)\frac{\partial W(\mathbf{p}, t)}{\partial \mathbf{p}} = -\sum_{\mathbf{p}'} [\gamma(p, p')W(\mathbf{p}, t) - \gamma(\mathbf{p}', \mathbf{p})W(\mathbf{p}', t)], \quad (87)$$

where $\mathbf{E}(t)$ is the vector of the external electric field, and

$$\gamma(\mathbf{p}, \mathbf{p}') = 2\pi Q^2(|\mathbf{p}-\mathbf{p}'|) \times \left[\frac{\delta\left(\frac{\mathbf{p}'^2}{2} - \frac{\mathbf{p}^2}{2} + 1\right)}{1-e^{-\beta}} + \frac{\delta\left(\frac{\mathbf{p}'^2}{2} - \frac{\mathbf{p}^2}{2} - 1\right)}{e^{\beta}-1}\right].$$

Such an equation describes electron scattering by optical phonons, i.e., it does not take into account the polaron effect. It was derived rigorously in Refs. 21 and 22 for the Fröhlich model in an electric field in the second order of perturbation theory [terms of order α^2 and $\alpha\mathbf{E}(t)$ are ignored]. Approximate solution of the Boltzmann equation[13] leads to the following expression for the electron drift mobility:

$$\mu = \frac{4e}{3\pi^{1/2}\alpha} G(\beta)(e^{\beta}-1)\beta^{-1/2}$$

as $\beta \to \infty$, $G(\beta) \to \frac{(3\pi\beta)^{1/2}}{8}$, and $\mu \to (e/2\alpha)e^{\beta}$; as $\beta \to 0$, $G(\beta) \to 1$ and $\mu \to \frac{4}{3}e\beta^{1/2}\alpha^{-1}\pi^{-1/2}$. There are various papers (Refs. 4, 44, 100, and 101) in which the Boltzmann description is generalized to the case of an arbitrary coupling constant α.

The results of Refs. 4, 100, and 101 predict that the polaron mobility increases with increasing coupling constant at sufficiently large α. Qualitatively, such a behavior is explained[102] by the strong screening of the polaron–phonon interaction, which for $\alpha \gg 1$ compensates the decrease in the mobility due to the increase in the effective polaron mass.

It is very difficult to establish clearly the limits of applicability of the Boltzmann approach in the case of intermediate or strong coupling. It is to be expected that it will hold at low temperatures, when the collision duration times (which are of order β) are much less than the relaxation time τ. At such temperatures, τ is very large and is determined by other scattering mechanisms. However, at the temperatures for which scattering by optical phonons is the main relaxation mechanism the Boltzmann-equation method is invalid.

Kubo's Method

In the case when not only perturbation theory but also the very method of using a Boltzmann equation is invalid, the polaron mobility can be calculated by means of Kubo's general formula

$$\mu = \frac{1}{2}e^2\beta\int_0^{\infty} dt\,\langle \hat{v}_i(0)\hat{v}_i(t) + \hat{v}_i(t)\hat{v}_i(0)\rangle, \quad (88)$$

where $\hat{v}_i(t)$ is the i-th component of the electron velocity operator in the Heisenberg representation. On the basis of (88), the calculation of the mobility reduces to determining the time correlation function of the velocities for a system in the state of thermodynamic equilibrium:

$$\langle \hat{v}_i(0)\hat{v}_i(t)\rangle = \frac{\mathrm{Tr}\, e^{-\beta\hat{H}}\hat{v}_i(0)\hat{v}_i(t)}{\mathrm{Tr}\, e^{-\beta\hat{H}}}.$$

Osaka[103] applied the expression (88) and the path-integral method to calculate the polaron mobility at low temperatures and an arbitrary coupling constant. He assumed that: a) the mobility is determined solely by the asymptotic behavior of the time correlation function $\langle \hat{v}_i(0)\hat{v}_i(t)\rangle$; b) this asymptotic behavior has the form of an exponential function of the time. His result agrees with the result of Ref. 100 obtained on the basis of a kinetic equation. A difficulty of Osaka's approach is that to make concrete calculations it is necessary to adopt additional and strong assumptions about the time dependence of the correlation functions, these evidently being equivalent to assuming the validity of a kinetic equation of Boltzmann type.

Kubo's expression (88) was also used in Ref. 104 by Langreth and Kadanoff to calculate the low-temperature polaron mobility in the fourth order of perturbation theory. They expressed the velocity correlation function in terms of the two-particle Green's function. The latter was then expanded in a series with respect to single-particle Green's functions and the electron–phonon interaction. Their result has the form

$$\mu = \frac{e}{2\alpha}\left(1 - \frac{\alpha}{6}\right)(e^{\beta}-1).$$

Note that for $\alpha \ll 1$ Osaka's formula for the mobility gives a very good approximation to this expression.

Nonequilibrium Density-Matrix Method

The most general expression for the polaron mobility at intermediate values of the coupling constant and the tem-

perature was obtained in Refs. 39 and 105 on the basis of an approximate calculation of the nonequilibrium density matrix of the electron–phonon system by the path-integral method. In Ref. 105, the mobility is obtained from the general expression for the polaron electrical conductivity $\sigma(\omega)$ in the limit $\omega \to 0$ (ω is the frequency of the external field), and in Ref. 39 from the expression for the steady velocity $\mathbf{v}(\mathbf{E})$ of an electron in an external constant electric field in the limit of weak fields. The result of Ref. 105 is

$$\mu^{-1} = \frac{\alpha e^{-1}}{3\sqrt{\pi}} \frac{\beta^{5/2} v^3}{\operatorname{sh} \beta/2} \times \int_0^\infty \frac{\cos u \, du}{\left[u^2 + \frac{\beta}{4} + \beta \frac{v^2-1}{Wv} \operatorname{cth} \frac{\beta W v}{2} - \frac{\beta (v^2-1)}{4} \frac{\cos Wvu}{\operatorname{sh} \frac{\beta W v}{2}}\right]^{3/2}}. \quad (89)$$

In the limit of very low temperatures, (89) leads to the expression

$$\mu = \frac{3}{2\beta} \frac{e}{2\alpha v^3} \exp\left\{\frac{v^2-1}{Wv} + \beta\right\},$$

which differs by the factor $3/2\beta$ from the expressions of Refs. 100 and 103. Since the result of Refs. 100 and 103 must be correct at least in the weak-coupling limit, it can be concluded that (89) leads to an incorrect temperature dependence of the polaron mobility in the limit $\beta \to \infty$. The reasons for this difference are as yet not entirely clear. In Ref. 105, the discrepancy was attributed to the invalidity of the employed approximations at $\omega = 0$. On the other hand, as was noted in Ref. 21, the approximate method used in Ref. 39 is equivalent to the assumption (when $\alpha \ll 1$) that the steady solution of the Boltzmann equation has the form of a Maxwell distribution with a certain mean velocity, and this assumption leads to an incorrect expression for the drift mobility at low temperatures. However, obscurity remains because (89) is obtained by two entirely independent methods.

6. CALCULATION OF POLARON ELECTRICAL CONDUCTIVITY BY THE PATH-INTEGRAL METHOD FOR THE DENSITY MATRIX

To overcome the shortcomings of the theory of electrotransport phenomena in polar crystals based on the Boltzmann equation and with the aim of creating a unified theory of the polaron impedance for arbitrary frequencies, temperatures, and coupling constants, Feynman, Hellwarth, Iddings, and Platzman (FHIP)[105] calculated the polaron linear response function by the nonequilibrium density-matrix method. For the linear response function, they obtained an exact representation in the form of a double path integral, which was then approximated in the framework of Feynman's one-oscillator model. The approach was developed further in Refs. 41, 75, 102, 106, and 107. The expressions obtained in this manner for the electrical conductivity make it possible to describe in a unified manner the polaron effects in optics, in galvanomagnetic phenomena, in cyclotron resonance, etc. The difficulties of the nonequilibrium density-matrix method are associated with the presence of a certain arbitrariness in the determination of the approximate expression for the impedance,[106,107] and this must be resolved on the basis of physically reasonable but mathematically nonrigorous considerations; they are also due to the fact that the method leads to an incorrect low-temperature dependence of the polaron drift mobility. An alternative approach that makes it possible to overcome the first of these difficulties is discussed below.

Expression for the Conductivity in Terms of the Response Function

An electron–phonon system in the presence of an external homogeneous electric field $\mathbf{E}(t)$ acting along the x axis is described by the Hamiltonian

$$\hat{H}(t) = \frac{\hat{\mathbf{p}}}{2} + eE(t)\, x + \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{+} \hat{a}_{\mathbf{k}} + e^{\varepsilon t} \sum_{\mathbf{k}} Q(k) \left[\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^{+}\right] e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (90)$$

The factor $e^{\varepsilon t}$ is introduced in order to achieve adiabatic switching-on of the interaction, and it corresponds to the limit $t_0 \to -\infty$, and then $\varepsilon \to 0^+$.

The nonequilibrium statistical operator $\hat{\rho}(t)$ of the system has the form

$$\hat{\rho}(t) = \hat{U}(E;\ t,\ t_0)\, \hat{\rho}(t_0)\, \hat{U}^{+}(E,\ t,\ t_0), \quad (91)$$

where $\hat{U}(E; t, t_0)$, the unitary operator of time evolution, satisfies the equation

$$i \frac{\partial}{\partial t} \hat{U}(E;\ t,\ t_0) = \hat{H}(t)\, \hat{U}(E;\ t,\ t_0);$$

$$t > t_0;\ \hat{U}(E;\ t_0,\ t_0) = 1.$$

Let $\langle x(t)\rangle_E$ be the mean value of the coordinate x of the electron at time t:

$$\langle x(t)\rangle_E = \operatorname{Tr}\{\hat{x}\hat{\rho}(t)\}.$$

The linear response function of the system is given by

$$Y(\tau - \sigma) = \frac{1}{e} \frac{\delta}{\delta E(\sigma)} \langle x(\tau)\rangle_{E=0},\ t_0 < \sigma < \tau,$$

and the conductivity $\sigma(\omega)$ can be expressed in terms of it by means of the formula

$$\sigma(\omega) = ie^2 \omega Y(\omega);$$
$$Y(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} Y(\tau);\ Y(\tau) = 0 \text{ for } \tau < 0, \quad (92)$$

where $Y(\omega)$ is the admittance of the system, an analytic function of ω for $\operatorname{Im}\omega > 0$.

To determine the function $Y(\tau - \sigma)$, it is sufficient to consider the response of the system to an external field $eE(s) = \xi\delta(s - \sigma)$. Then

$$Y(\tau - \sigma) = \frac{\partial}{\partial \xi} \langle x(\tau)\rangle_{\xi=0}.$$

We now consider the generating function

$$g(\xi,\ \eta) = \operatorname{Tr}\{\hat{U}(E;\ t,\ t_0)\, \hat{\rho}(t_0)\, \hat{U}^{+}(E';\ t,\ t_0)\}, \quad (93)$$

where

$$E(s) = \xi\delta(s - \sigma) + \eta\delta(s - \tau);$$

$$E'(s) = \xi\delta(s-\sigma) - \eta\delta(s-\tau), \quad t_0 < \sigma < \tau < t.$$

It is readily seen that

$$\langle x(t)\rangle_\xi = \frac{i}{2}\frac{\partial}{\partial\eta} g(\xi, \eta)\Big|_{\eta=0},$$

and for $Y(\tau-\sigma)$ we then have

$$Y(\tau-\sigma) = \frac{i}{2}\frac{\partial^2}{\partial\xi\,\partial\eta} g(\xi, \eta)\Big|_{\xi=\eta=0}. \quad (94)$$

Thus, the calculation of the electrical conductivity reduces to finding the function $g(\xi, \eta)$ in terms of which $Y(\tau-\sigma)$ is expressed.

Path-Integral Representation for the Generating Function

To obtain an expression for $g(\xi, \eta)$ in the form of a path integral, we rewrite (93) in the form

$$g(\xi, \eta) = \int\int\int\int\int\int d^3\mathbf{r}\, d^3\mathbf{r}'\, d^3\mathbf{r}''\, dQ\, dQ'\, dQ''$$
$$\times \langle \mathbf{r}, Q | \hat{U}(E; t, t_0) | \mathbf{r}', Q'\rangle \langle \mathbf{r}', Q' | \hat{\rho}(t_0) | \mathbf{r}'', Q''\rangle$$
$$\times \langle \mathbf{r}, Q | \hat{U}(E'; t, t_0) | \mathbf{r}'', Q''\rangle^*. \quad (95)$$

Then, using the Feynman–Kac formula for the matrix elements $\langle \mathbf{r}, Q | \hat{U}(E; t, t_0) | \mathbf{r}', Q'\rangle$, we obtain

$$\langle \mathbf{r}, Q | \hat{U}(E; t, t_0) | \mathbf{r}', Q'\rangle$$
$$= \int_{\mathbf{x}(t_0)=\mathbf{r}'}^{\mathbf{x}(t)=\mathbf{r}} D\mathbf{x} \int_{Q(t_0)=Q'}^{Q(t)=Q} DQ \exp\left\{-i\int_{t_0}^{t} d\tau H[\tau, \mathbf{x}(\tau), Q(\tau)]\right\}.$$

For $t = t_0$, when the electric field has not yet acted [we consider the response of the system to the field $eE(s) = \xi\delta(s-\sigma)$] and the electron has not interacted with the phonons, $e^{\varepsilon t_0} \to 0$ as $t_0 \to -\infty$, it is natural to assume that the phonon subsystem is in the Gibbs state of thermodynamic equilibrium at temperature T. The choice of the initial conditions for the electron is to a certain degree arbitrary, but the most convenient assumption is that the electron is in a state with a completely uncertain value of the momentum. Then

$$\langle \mathbf{r}', Q' | \hat{\rho}(t_0) | \mathbf{r}'', Q''\rangle = \delta(\mathbf{r}'-\mathbf{r}'') \frac{\langle Q' | e^{-\beta\hat{H}}\mathbf{F} | Q''\rangle}{\int dQ \langle Q | e^{-\beta\hat{H}}\mathbf{F} | Q\rangle},$$

whence

$$\langle \mathbf{r}', Q' | \hat{\rho}(t_0) | \mathbf{r}'', Q''\rangle$$
$$= \delta(\mathbf{r}'-\mathbf{r}'') \frac{\int_{Q(0)=Q''}^{\zeta(\beta)=Q'} DQ \exp\left\{-\frac{1}{2}\sum_{\mathbf{k}}\int_0^\beta d\tau [\dot{q}_{\mathbf{k}}^2(\tau) + q_{\mathbf{k}}^2(\tau)]\right\}}{\int_{Q(0)=Q(\beta)} DQ \exp\left\{-\frac{1}{2}\sum_{\mathbf{k}}\int_0^\beta d\tau [\dot{q}_{\mathbf{k}}^2(\tau) + q_{\mathbf{k}}^2(\tau)]\right\}}.$$

The Gaussian path integrals which occur here can be readily calculated (see Refs. 102 and 105), and the result is

$$\langle \mathbf{r}', Q' | \hat{\rho}(t_0) | \mathbf{r}'', Q''\rangle = \delta(\mathbf{r}'-\mathbf{r}'') \prod_{\mathbf{k}} \left(\frac{\operatorname{th}\beta/2}{\pi}\right)^{1/2}$$
$$\times \exp\left\{-\frac{1}{2\operatorname{sh}\beta}\left[\left(q_{\mathbf{k}}' + q_{\mathbf{k}}''\right)^2 \operatorname{ch}\beta - 2q_{\mathbf{k}}' q_{\mathbf{k}}''\right]\right\}.$$

To obtain the final expression for $g(\xi, \eta)$ we must now:

a) integrate over the paths of the oscillators in the expressions for $\langle \mathbf{r}, Q | \hat{U}(E; t, t_0) | \mathbf{r}', Q'\rangle$ and $\langle \mathbf{r}, Q | \hat{U}(E'; t, t_0) | \mathbf{r}'', Q''\rangle$ by means of expressions of the type (9) (see Refs. 102 and 105);

b) integrate over Q, Q', and Q'' in (95);

c) make the change of variables $\mathbf{x}(s) = \mathbf{r}(t-s)$.

Then in the limit $t_0 \to -\infty$ we obtain

$$g(\xi, \eta) = \int_{\mathbf{r}(0)=\mathbf{r}'(0)}^{\mathbf{r}(\infty)=\mathbf{r}'(\infty)}\int\int D\mathbf{r}D\mathbf{r}' e^{i\Phi(\mathbf{r}, \mathbf{r}')}, \quad (96)$$

where

$$\left.\begin{aligned}
&\Phi(\mathbf{r}, \mathbf{r}') \\
&= \int_0^\infty dt\left\{\frac{1}{2}[\dot{\mathbf{r}}^2(t) - \dot{\mathbf{r}}'^2(t)] + E(t)x(t) - E'(t)x'(t)\right\} \\
&\quad + V(\mathbf{r}) - V^*(\mathbf{r}') + U(\mathbf{r}, \mathbf{r}'); \\
&V(\mathbf{r}) \\
&= i\sum_{\mathbf{k}} Q^2(k)\int_0^\infty dt\int_0^t ds\, e^{-\varepsilon(t+s)} C[i(t-s)]\, e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(s)]}; \\
&U(\mathbf{r}, \mathbf{r}') \\
&= -i\sum_{\mathbf{k}} Q^2(k)\int_0^\infty\int_0^\infty dt\, ds\, e^{-\varepsilon(t+s)} C[i(t-s)]\, e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}'(s)]}.
\end{aligned}\right\} \quad (97)$$

The integral in (96) is normalized in such a way that $g(\xi, 0) = 1$. The expression (96) represents a significant simplification of the problem compared with (93), since the phonon variables have been exactly eliminated. The outcome of the elimination is an effective electron–electron interaction described by the functionals $V(\mathbf{r})$, $V^*(\mathbf{r}')$, and $U(\mathbf{r}, \mathbf{r}')$. The physical meaning of these terms is discussed in detail in Ref. 70. In particular, it is shown that $U(\mathbf{r}, \mathbf{r}')$ is responsible for dissipation.

The expressions (92), (94), (96), and (97) can be readily generalized to the case when the conduction electron is characterized by a tensor effective mass $\hat{m}$, the system is subject to a magnetic field $\mathbf{h}$, and the electron interacts with several branches of the phonon spectrum, each of which is characterized by a dispersion law $\omega_n(\mathbf{k})$.[40,41,75,106] The Hamiltonian of the system in this case has the form

$$\hat{H} = \frac{1}{2}\left(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}\right)\frac{1}{\hat{m}}\left(\hat{p} + \frac{e}{c}\mathbf{A}\right) + e\mathbf{E}(t)\cdot\mathbf{r}$$
$$+ \sum_{n,\,k}\{\omega_n(\mathbf{k})\hat{a}_{\mathbf{k},\,n}^+\hat{a}_{\mathbf{k},\,n} + Q_n(\mathbf{k})[\hat{a}_{\mathbf{k},\,n} + \hat{a}_{-\mathbf{k},\,n}^+]\, e^{i\mathbf{k}\cdot\mathbf{r}}\}, \quad (98)$$
$$\mathbf{A} = \frac{1}{2}(\mathbf{h}\times\mathbf{r}).$$

Then

$$\sigma_{ik} = ie^2\omega Y_{ik}(\omega);$$

$$Y_{ik}(\tau-\sigma) = \frac{i}{2}\frac{\partial^2}{\partial\xi_k\,\partial\eta_i} g(\xi, \eta)\Big|_{\xi=\eta=0}$$

and $g(\xi, \eta)$ is determined by the expression (96), in which we now have

$$\Phi(\mathbf{r},\ \mathbf{r}')=\int_0^\infty dt\left\{\frac{1}{2}[\dot{\mathbf{r}}(t)\cdot\overleftrightarrow{m}\cdot\dot{\mathbf{r}}(t)-\dot{\mathbf{r}}'(t)\cdot\overleftrightarrow{m}\cdot\dot{\mathbf{r}}'(t)]+\right.$$
$$+\mathbf{E}(t)\,\mathbf{r}(t)-\mathbf{E}'(t)\cdot\mathbf{r}'(t)+\frac{e}{2c}[\dot{\mathbf{r}}(t)\cdot(\mathbf{r}(t)\times\mathbf{h})-$$
$$\left.-\dot{\mathbf{r}}'(t)\cdot(\mathbf{r}'(t)\times\mathbf{h})]\right\}+V(\mathbf{r})-V^*(\mathbf{r}')+U(\mathbf{r},\ \mathbf{r}');$$
$$V(\mathbf{r})=\mathrm{i}\sum_{n,\ \mathbf{k}}Q_n^2(\mathbf{k})\int_0^\infty dt\int_0^t ds\,\mathrm{e}^{-\varepsilon(t+s)}\times$$
$$\times C_{\omega_n(\mathbf{k})}[\mathrm{i}(t-s)]\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(s)]};$$
$$U(\mathbf{r},\ \mathbf{r}')=-\mathrm{i}\sum_{n,\ \mathbf{k}}Q_n^2(\mathbf{k})\int_0^\infty dt\int_0^\infty ds\,\mathrm{e}^{-\varepsilon(t+s)}\times$$
$$\times C_{\omega_n(\mathbf{k})}[\mathrm{i}(t-s)]\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}'(s)]}. \tag{99}$$

Such a representation for the total nonequilibrium statistical operator (98) of the system $\langle\mathbf{r}Q|\hat{\rho}(t)|\mathbf{r}',Q'\rangle$ was obtained in Ref. 108 for an arbitrary choice of the initial distribution $\hat{\rho}(t_0)$.

Approximate Expression for the Conductivity

For the approximate calculation of $g(\xi,\eta)$ on the basis of (96) it is necessary to approximate $\Phi(\mathbf{r},\mathbf{r}')$ by a functional $\Phi_0(\mathbf{r},\mathbf{r}')$ for which the path integrals of the type (96) can be calculated exactly. With allowance for the first correction (due to the difference between Φ and Φ_0),

$$\mathrm{e}^{\mathrm{i}\Phi}=\mathrm{e}^{\mathrm{i}\Phi_0+\mathrm{i}(\Phi-\Phi_0)}\simeq\mathrm{e}^{\mathrm{i}\Phi_0}[1+\mathrm{i}(\Phi-\Phi_0)];$$
$$g(\xi,\ n)\simeq g_0(\xi,\ \eta)[1+\mathrm{i}\langle\Phi-\Phi_0\rangle_{\Phi_0}], \tag{100}$$

where

$$g_0(\xi,\ \eta)=\int_{\mathbf{r}(0)=\mathbf{r}'(0)}^{\mathbf{r}(\infty)=\mathbf{r}'(\infty)}\int D\mathbf{r}D\mathbf{r}'\mathrm{e}^{\mathrm{i}\Phi_0(\mathbf{r},\ \mathbf{r}')}.$$

The most general choice of Φ_0 corresponds to replacement of the functionals $V(\mathbf{r})$, $V^*(\mathbf{r})$, and $U(\mathbf{r},\mathbf{r}')$ in (97) by quadratic functionals. We have

$$\Phi_0(\mathbf{r},\ \mathbf{r}')=\int_0^\infty dt\left\{\frac{1}{2}[\dot{\mathbf{r}}^2(t)-\dot{\mathbf{r}}'^2(t)]\right.$$
$$\left.+E(t)\,x(t)-E'(t)\,x'(t)\right\}$$
$$+V_0(\mathbf{r})-V_0^*(\mathbf{r}')+U_0(\mathbf{r},\ \mathbf{r}');$$
$$V_0(\mathbf{r})=-\mathrm{i}\int_{-\infty}^\infty dWG(W)\int_0^\infty dt\int_0^t ds\,\mathrm{e}^{-\varepsilon(t+s)}\mathrm{e}^{\mathrm{i}W(t-s)}$$
$$\times|\mathbf{r}(t)-\mathbf{r}(s)|^2;$$
$$U_0(\mathbf{r},\ \mathbf{r}')=\mathrm{i}\int_{-\infty}^\infty dWG(W)\int_0^\infty dt\int_0^\infty ds\,\mathrm{e}^{-\varepsilon(t+s)}\mathrm{e}^{\mathrm{i}W(t-s)}$$
$$\times|\mathbf{r}(t)-\mathbf{r}'(s)|^2. \tag{101}$$

The functional $\Phi_0(\mathbf{r},\mathbf{r}')$ corresponds to a system in which the electron interacts with a distribution of oscillators of all possible frequencies.

For such a choice of Φ_0, the path integrals in (100) can be readily calculated (see Refs. 102 and 105) and the admittance is found to be

$$Y(\omega)=Y_0(\omega)\left[1+\frac{Z_1(\omega)}{Z_0(\omega)}\right], \tag{102}$$

where $Z_0(W)=Y_0^{-1}(\omega)$ is the impedance of the model (101):

$$Z_0(\omega)=\omega^2\left[1+4\int_{-\infty}^\infty dW\frac{P}{W}\frac{G(W)}{W^2-\omega^2-\mathrm{i}\varepsilon}\right],$$
$$Z_1(\omega)=-\omega^2+Z_0(\omega)+\chi(\omega);$$
$$\chi(\omega)=\frac{2\alpha}{3\sqrt{\pi}}\int_0^\infty du(1-\mathrm{e}^{\mathrm{i}\omega u})\,\mathrm{Im}\,[C(-\mathrm{i}u)D^{-3/2}(u)];$$
$$D(u)=4\int_{-\infty}^\infty d\omega\frac{G(\omega)}{Z_0(\omega)Z_0^*(\omega)}(1-\mathrm{e}^{\mathrm{i}\omega u}). \tag{103}$$

The generalization of these expressions to the case of an anisotropic crystal in the presence of a magnetic field and interaction of the electron with several branches of the phonon spectrum is not difficult and was done in Refs. 40, 41, 75 and 106.

The expression (102) is an expansion of the admittance. However, the conductivity $\sigma(\omega)$ obtained from (92) and (102) does not exhibit the expected resonance behavior and depends very strongly on the choice of the zeroth approximation Y_0. As is shown in Ref. 105, from the physical point of view expansion of the impedance $Z(\omega)=Y^{-1}(\omega)$ is much more meaningful. From (102),

$$Z(\omega)=\frac{Z_0(\omega)}{1+Z_1(\omega)/Z_0(\omega)}.$$

Then, if $Z_1(\omega)/Z_0(\omega)\ll 1$,

$$Z(\omega)=Z_0(\omega)-Z_1(\omega)=\omega^2-\chi(\omega). \tag{104}$$

It is the expression (104) that is taken as the approximate expression for the polaron impedance. The conductivity $\sigma(\omega)=ie^2\omega/Z(\omega)$ obtained by means of (104) has the expected resonance behavior. The first term on the right-hand side of (104) is the purely inductive term characteristic of a free particle. The second term takes into account the influence of the finite lifetime due to the electron–phonon coupling.

In the special case when the approximating functional Φ_0 is taken to be the functional of the linear model (18) [or Feynman's one-oscillator model (16)], the function $D(u)$ takes the form given by Feynman *et al.*[105]:

$$D(u)=\frac{1}{v^2}\left\{-\mathrm{i}u+\frac{u^2}{\beta}\right.$$
$$\left.+\frac{v^2-1}{Wv}\frac{1-\mathrm{e}^{\mathrm{i}Wvu}-\mathrm{e}^{-Wv(\mathrm{i}u+\beta)}+\mathrm{e}^{-\beta Wv}}{1-\mathrm{e}^{-\beta Wv}}\right\}. \tag{105}$$

In Ref. 75, an approximating functional Φ_0 of a form somewhat different from (101) was used in a study of the polaron electrical-conductivity tensor in a magnetic field.

The results of Klyukanov and Pokatilov are valid for all frequencies and magnetic field strengths, but only for a weak electron–phonon coupling. In the limit $\omega_c\to 0$ ($h\to 0$) they

agree with the result of Ref. 105 [if one sets $\nu = 1$ in that result ($\alpha \ll 1$)].

Frequency and Temperature Dependence of the Polaron Conductivity

The expressions (92), (103), and (104) and their generalization to the case when a uniform magnetic field acts on the system[41,75,106,107] make it possible to study the behavior of the polaron conductivity for arbitrary values of the parameters α, β, ω, and h. We shall summarize the main information obtained from these expressions.

a) Reactive Part of the Impedance. Effective Mass

At zero temperature ($\beta \to \infty$) and $\omega < 1$ it follows from (103) and (104) that the polaron impedance is a real quantity and is given by

$$Z(\omega) = \omega^2 \left\{ 1 - \frac{2\alpha\nu^3}{3\sqrt{\pi}\,\omega^2} \int_0^\infty \frac{dt e^{-t}(1-\operatorname{ch}\omega t)}{\left[t + \frac{\nu^2-1}{W\nu}(1-e^{-W\nu t}) \right]^{3/2}} \right\}. \tag{106}$$

Thus, for $\omega < 1$ and $\beta = \infty$, when there are no thermal phonons that could scatter the polaron and decelerate its motion, the polaron is accelerated without dissipation under the influence of the applied field. If there exist phonons with zero frequency such as long-wavelength acoustic phonons, the resistivity is also finite at zero temperature. Since only the interaction of the electron with the longitudinal optical phonons is taken into account in the Pekar–Fröhlich model, a polaron resistivity appears at $\omega = 1$. Of course, in a constant field a polaron ultimately acquires sufficient energy to emit one optical phonon and thus dissipate energy, but this effect is nonlinear in the field and is not described in linear response theory. At very low frequencies, the expression (106) goes over into

$$Z(\omega) = -m_F^*(\alpha)\,\omega^2, \tag{107}$$

where the effective mass $m_F^*(\alpha)$ is determined by (51). Thus, at zero temperature and low frequencies of the external field the polaron behaves like a particle with mass $m_F^*(\alpha)$.

In the general case of finite temperatures we obtain for Re $Z(\omega)$ and Im $Z(\omega)$ the expressions[105]

$$\operatorname{Im} Z(\omega) = \frac{2\alpha\nu^3}{3\sqrt{\pi}} \frac{\operatorname{sh}\frac{\beta\omega}{2}}{\operatorname{sh}\beta/2} \times \int_0^\infty \frac{dt \cos t \cos\omega t}{\left\{ \frac{t^2}{\beta} + \frac{\beta}{4} + \frac{\nu^2-1}{W\nu}\left[\frac{\operatorname{ch}\frac{\beta W\nu}{2} - \cos W\nu t}{\operatorname{sh}(\beta W\nu/2)} \right] \right\}^{3/2}};$$

$$\operatorname{Re} Z(\omega) = \omega^2 - \frac{2\alpha\nu^3}{3\sqrt{\pi}} \times \int_0^{\beta/2} \frac{d\tau\,[1-\operatorname{ch}\omega\tau]\,C(\tau)}{\left[\tau\left(1-\frac{\tau}{\beta}\right) + \frac{\nu^2-1}{W\nu}\frac{1-e^{-W\nu\tau}-e^{-W\nu(\beta-\tau)}+e^{-\beta W\nu}}{1-e^{-\beta W\nu}} \right]^{3/2}}$$

$$+ \frac{2\alpha\nu^3}{3\sqrt{\pi}} \frac{\operatorname{sh}\frac{\beta\omega}{2}}{\operatorname{sh}\beta/2} \int_0^\infty \frac{dt \cos t \sin\omega t}{\left[\frac{t^2}{\beta} + \frac{\beta}{4} + \frac{\nu^2-1}{W\nu}\frac{\operatorname{ch}\frac{\beta W\nu}{2} - \cos W\nu t}{\operatorname{sh}\frac{\beta W\nu}{2}} \right]^{3/2}}.$$

For a free particle of mass M and lifetime τ the impedance is

$$Z(\omega) = \frac{iM\omega}{\tau} + M\omega^2.$$

Then for the polaron when $\beta \gg 1$ and $\omega \ll 1$

$$M = 1 + \frac{\alpha\nu^3}{3\sqrt{\pi}} \int_0^{\beta/2} dt \frac{t^2 e^{-t}}{\left[t\left(1-\frac{t}{\beta}\right) + \frac{\nu^2-1}{W\nu}(1-e^{-W\nu t}) \right]^{3/2}};$$

$$\tau = \lim_{\omega\to 0} \frac{\operatorname{Im} Z(\omega)}{\omega \operatorname{Re} Z(\omega)} = M \lim_{\omega\to 0} \frac{\omega}{\operatorname{Re} Z(\omega)}.$$

The expression for M is identical to the expression (72) for the effective polaron mass at low temperatures. At higher temperatures, an important contribution is also made by the term in the expression for Re $Z(\omega)$ proportional to $\frac{\operatorname{sh}\beta\omega/2}{\sin\beta/2}$. The corresponding expression for the effective mass is then identical to the expression obtained in Ref. 75 for the case of weak coupling. However, with increasing temperature the lifetime τ decreases very strongly, and the quasiparticle picture ceases to hold.

b) Polaron Mobility

The polaron mobility is expressed in terms of Re $Z(\omega)$ by[105]

$$\mu^{-1} = \lim_{\omega\to 0} \frac{\operatorname{Im} Z(\omega)}{e\omega} = \frac{\alpha\beta^{5/2}\nu^3}{3e\sqrt{\pi}\operatorname{sh}\beta/2} \times \int_0^\infty \frac{\cos u\,du}{\left[u^2 + \frac{\beta^2}{4} + \beta\frac{\nu^2-1}{W\nu}\frac{\operatorname{ch}\frac{\beta W\nu}{2} - \cos W\nu t}{\operatorname{sh}\frac{\beta W\nu}{2}} \right]^{3/2}}.$$

At low temperatures ($\beta \to \infty$)

$$\tau = \frac{3}{2\beta}\frac{e}{2\alpha\nu^3}\exp\left\{ \frac{\nu^2-1}{W\nu} + \beta \right\},$$

and at high temperatures ($\beta \to 0$, $\nu \to 1$)

$$\mu = \frac{3\sqrt{\pi}}{8}\frac{e\beta^{1/2}}{\alpha}.$$

In the weak-coupling limit and for arbitrary temperature,

$$\mu = \frac{3e\sqrt{\pi}\operatorname{sh}\beta/2}{2\alpha\beta^{3/2}K_1(\beta/2)},$$

where $K_1(z)$ is a cylindrical function of an imaginary argument.

As we have already noted, the mobility obtained in Ref. 105 at low temperatures differs by the factor $3/2\beta$ from the generally accepted expression for the low-temperature po-

laron mobility. The reason is evidently that the expansion (104) for the impedance is not valid at $\omega = 0$. We note, however, that the expression (89), which is physically reasonable for all values of α and β, is obtained in two independent ways and leads to the correct temperature dependence of the mobility as $\beta \to 0$ ($\mu \sim \beta^{1/2}$).

c) Polaron Effects in the Optical Region of the Spectrum

The frequency dependence of the impedance obtained in Ref. 105 is particularly interesting, since it exhibits a strong dispersion, the nature of this dispersion depending primarily on α for frequencies larger than 1. To find the dispersion at zero temperature, it is convenient to expand the expression for Im $Z(\omega)$ in powers of the parameter $R = (\nu^2 - 1)/W\nu$. We then find[107]

$$\operatorname{Im} Z(\omega) = \frac{2\alpha\nu^3}{3\sqrt{\pi}} \sum_{n=0}^{\infty} C_n^{-3/2} (-1)^n \frac{R^n 2^n}{(2n+1)!!} \times (\omega - 1 - nW\nu)^{n+1/2}\, \theta(\omega - 1 - nW\nu)\, e^{-R(\omega-1-nW\nu)}, \quad (108)$$

where $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ if $x < 0$, and $C^{-3/2}$ are known numerical coefficients. For fixed frequency ω, this expression is a finite quantity. The first two terms of this sum were obtained for the first time in Ref. 105. The first threshold in Im $Z(\omega)$ appears at $\omega = 1$ and corresponds to the absorption of one quantum of the electromagnetic field with the emission of one optical phonon. The next threshold appears at $\omega = 1 + W\nu$ and corresponds to transition of a polaron to an excited state of energy $E_0 + W\nu$ with emission of one optical phonon. The interpretation of the thresholds that appear at $\omega = 1 + nW\nu$ is similar. We may recall here that in his variant of strong-coupling theory Pekar[1] found that the energy of the lowest excited state is $0.1395\alpha^2$, and in Feynman's theory $W\nu = \frac{4\alpha^2}{9\pi} = 0.1415\alpha^2$ for $\alpha \gg 1$. In the case of strong coupling, the electron is localized in the polarization well which it creates. The excited states of this well are not stationary, since after an optical transition the atoms of the lattice will move to new equilibrium positions. In this excited state, the electron has a finite lifetime, which increases with increasing α, and the electron relaxes to a different excited state corresponding to the new equilibrium position of the ions. In the literature, these excited states have become known as Franck–Condon and relaxed (or self-consistent) states, respectively. The energies, masses, and radii of the relaxed excited polaron states were calculated in the strong-coupling limit in Ref. 109. In the interpretation of Ref. 105, the thresholds in the frequency dependence Im $Z(\omega)$ correspond to transitions to Franck–Condon states, while the relaxed states are not observed. The maxima in Im $Z(\omega)$ that appear when ω becomes equal to the energies of these unstable excited states are broadened by virtue of their short lifetime against phonon emission. With increasing α, the number of maxima in Im $Z(\omega)$ increases, and the widths decrease. For not too strong coupling, $\alpha \leqslant 3$, the lifetime effects wash out the threshold structure, and there remains only the single-phonon peak at $\omega \gtrsim 1$. Thus, if threshold structure is to be observed in Im $Z(\omega)$ it is necessary for α to be of order 5 or more.

However, as was shown in Refs. 107 and 110, the optical absorption spectrum of free polarons is determined not only by the function Im $Z(\omega)$ but also depends on the reactive part Re $Z(\omega)$. Indeed, the coefficient of optical absorption $\Gamma(\omega)$ is proportional to Re $\sigma(\omega)$, which depends on both Re $Z(\omega)$ and Im $Z(\omega)$:

$$\Gamma(\omega) \sim \operatorname{Re}\sigma(\omega) = \frac{e^2\omega \operatorname{Im} Z(\omega)}{[\operatorname{Re} Z(\omega)^2 + \operatorname{Im} Z(\omega)]^2}.$$

The frequency dependence $\Gamma(\omega)$ for $\beta = \infty$ was investigated in Refs. 107 and 110. In the case $\alpha < 1$, analytic calculations lead to the results of Ref. 111 obtained in perturbation theory, and the absorption spectrum is characterized by a sharp single-phonon peak at $\omega \gtrsim 1$.

Numerical calculations for $\alpha = 1, 3, 5, 6, 7, 11$ show that the structure of $\Gamma(\omega)$ is more complicated than the frequency dependence of Im $Z(\omega)$. Sharp peaks at frequencies $\omega \lesssim W\nu$ appear together with broad maxima at $\omega \gtrsim W\nu$ when α takes the values 5, 6, 7, 11. They are interpreted as transitions to relaxed and Franck–Condon states, respectively. For $\alpha \gg 1$, the behavior of $\Gamma(\omega)$ agrees qualitatively with the results of Ref. 112. Note that the single-phonon peak predicted by weak-coupling theory was observed in CdO,[113] but structures associated with excited states of free polarons have not yet been observed. However, for polarons bound in a Coulomb potential, transitions to excited states lead to the appearance of additional lines in the spectrum of light absorption.[114,115]

d) Cyclotron Resonance and Galvanomagnetic Phenomena

Generalization of the results of Ref. 105 to the case of an anisotropic electron interacting with different phonon modes in the presence of a constant magnetic field **h** makes it possible to study cyclotron resonance of polarons and investigate the behavior of the magnetoresistivity, the Hall mobility, and other observable quantities. The most general expressions for the impedance $\overleftrightarrow{Z}(\omega)$ were obtained by Thornber[41] and have the form

$$\left.\begin{aligned}
&\overleftrightarrow{Z}(\omega) = \overleftrightarrow{m}\omega^2 + \frac{ie\omega}{c}\epsilon\cdot\mathbf{h} - \int_0^\infty dt\,(1 - e^{i\omega t})\operatorname{Im}\overleftrightarrow{S}(t);\\
&S_{ij}(t) = 2\sum_{n,\mathbf{k}} k_i k_j Q_n^2(\mathbf{k})\, C_{\omega n(\mathbf{k})}\,(-it)\, e^{-\frac{1}{2}\mathbf{k}\cdot\overleftrightarrow{D}(t)\cdot\mathbf{k}};\\
&\overleftrightarrow{D}(t) = 4\int_{-\infty}^{\infty} d\omega \frac{1}{\overleftrightarrow{Z_0}(\omega)}\overleftrightarrow{G}(-\omega)\frac{1}{\overleftrightarrow{Z_0^+}(\omega)}(1 - e^{-i\omega t});\\
&\overleftrightarrow{Z_0}(\omega) = \overleftrightarrow{m}\omega^2 + i\frac{e}{c}\omega\epsilon\cdot\mathbf{h} + 4\omega^2\int_{-\infty}^{\infty} dW \frac{P}{W}\frac{\overleftrightarrow{G}(W)}{W^2 - \omega^2 - i\varepsilon},
\end{aligned}\right\} \quad (109)$$

where ϵ is the completely antisymmetric tensor of rank 3.

For an optical polaron in the case of an anisotropic conduction band and magnetic field directed along the z axis, the most general choice of $\overleftrightarrow{G}(W)$ is

$$G_{ij}(W) = G_j(W)\,\delta_{ij};\ G_1(W) = G_2(W) = G_\perp(W).$$

Then the impedance tensor is

$$Z_{jj}(\omega,\ \omega_c) = \frac{iM_j\omega}{\tau_j}(1 - i\omega\tau_j);\quad Z_{12}(\omega,\ \omega_c) = -Z_{21}(\omega,\ \omega_c) = i\omega\omega_c^* M_\perp;$$
$$Z_{13} = Z_{23} = Z_{31} = Z_{32} = 0,$$

where

$$\omega_c^* = \frac{eh}{cM_\perp};\quad M_1 = M_2 = M_\perp;\quad \tau_1 = \tau_2 = \tau_\perp;$$

$$M_i(\omega,\ \omega_c) = 1 - \frac{1}{\omega^2}\,\mathrm{Im}\int_0^\infty dt\,(1 - \cos\omega t)\,S_i(t);$$

$$S_i(t) = 2\sum_{\mathbf{k}} Q^2(k)\,k_i^2 C(-it) \times \exp\left\{-\frac{1}{2}(k_1^2 + k_2^2)\,D_\perp(t) - \frac{1}{2}k_3^2 D_3(t)\right\};$$

$$Z_{ii}^0(\omega,\ \omega_c) = \omega^2\left\{1 + 4\int_{-\infty}^{\infty} dW\,\frac{P}{W}\,\frac{G_i(W)}{W^2 - \omega^2 - i\varepsilon}\right\};$$

$$Z_{12}^0 = -Z_{21}^0 = i\omega\omega_c.$$

The results of Ref. 75 are obtained for $G_i(W) = 0$. The cyclotron resonance frequency is determined by the maximum of $\mathrm{Re}\,\sigma_\perp(\omega, \omega_c)$. If the magnetic field is weak, then $\omega_c^* \ll 1$, and the frequency dependence of $\tau_\perp(\omega, \omega_c)$ and $M_\perp(\omega, \omega_c)$ can be ignored. Then the maximum is attained at

$$(\omega/\omega_c^*)^2 = 1 - 1/(\omega_c^*\tau)^2.$$

At low temperatures ($e^\beta \gg 1$), $\omega_c^*\tau_\perp \gg 1$ and the cyclotron resonance frequency is ω_c^*. Then the cyclotron mass is $m_c = M_\perp(\omega_c^*, \omega_c)$ and differs from the effective polaron mass $M(\alpha, \beta)$ (72) only by the dependence on the magnetic field. However, since $\omega_c^* < \omega_c \ll 1$,

$$m_c = M + O(\omega_c^2).$$

At higher temperatures ($\beta \gtrsim 1$), the condition $\omega_c^*\tau_\perp \gg 1$ is not satisfied. The cyclotron resonance frequency differs from ω_c^*, and the cyclotron mass m_c is not equal to $M_\perp(\omega_c^*, \omega_c)$. We have

$$m_c = \frac{M_\perp(\omega_c^*,\ \omega_c)}{\sqrt{1 - (\omega_c^*\tau)^{-2}}} \simeq M_\perp(0,\ 0)\left\{1 + \frac{1}{2(\omega_c^*\tau_\perp)^2} + \ldots\right\};$$
$$\omega_c^* < \omega_c \ll 1.$$

In contrast to the parameter $M_\perp(0, 0)$, the cyclotron mass m_c is always greater than unity. Therefore, the negative polaron effect obtained in Ref. 75 [$M_\perp(0, 0) < 1$ for $\beta \gtrsim 1$] should not hold for the cyclotron mass m_c if one could succeed in observing cyclotron resonance of polarons at such temperatures.

The magnetoresistivity $\overleftrightarrow{\rho}(\omega_c)$ is determined by the impedance $\overleftrightarrow{Z}(\omega, \omega_c)$ through

$$\overleftrightarrow{\rho}(\omega_c) = \lim_{\omega\to 0}\frac{\overleftrightarrow{Z}(\omega,\ \omega_c)}{ie^2\omega}.$$

Then for the longitudinal, $\rho_{33}(\omega_c)$ and transverse, $\rho_\perp(\omega_c)$, magnetoresistivity we have

$$\rho_{33}(\omega_c) = \frac{M_3(0,\ \omega_c)}{e^2\tau_3(0,\ \omega_c)};\quad \rho_\perp(\omega_c) = \frac{M_\perp(0,\ \omega_c)}{e^2\tau_\perp(0,\ \omega_c)}.$$

In Ref. 41, the behavior of ρ_{33} and $\rho_\perp$ in the case of weak fields ($\omega_c \ll 1$) is considered, and it is found that

$$\rho_{33}(\omega_c) = \rho_0 + r_\parallel\omega_c^2,\quad \rho_\perp(\omega_c) = \rho_0 + r_\perp\omega_c^2,$$

where ρ_0 is the resistivity in the absence of the magnetic field and $r_\parallel = \frac{1}{2}r_\perp$.

In Ref. 75, the behavior of the longitudinal and transverse magnetoresistivity was studied in the case of weak coupling and a strong magnetic field ($\omega_c \sim 1$). The longitudinal magnetoresistivity at low temperatures consists of a nonoscillating and an oscillating part. The nonoscillating part increases linearly with ω_c, in agreement with experiment. The oscillating part is small and has a maximum at $\omega_c = 1$. Oscillations of the longitudinal magnetoresistivity in strong fields are also observed in experiments in polar crystals.[116] The transverse resistivity exhibits resonance oscillations. Because of the neglect of the dispersion of the optical phonons and other mechanisms that limit the height of the oscillations, $\rho_\perp(\omega_c)$ diverges logarithmically at the points $\omega_c = 1/N$. The results of Ref. 75 agree with those obtained in Ref. 117 by perturbation theory.

The magnetic-field dependence of the magnetoresistivity is due to the influence of the field on electron scattering by optical phonons. Since the electron is scattered in all directions, the magnetic field influences the resistivity for an electron moving both in the direction of the field and perpendicular to it. The conductivity, the reciprocal of the resistivity, has a further, kinematic dependence on the field:

$$\sigma_\perp(\omega_c) = \frac{e^2\tau_\perp(0,\ \omega_c)}{M_\perp(0,\ \omega_c)}\,\frac{1}{1 + \omega_c^{*2}\tau_\perp^2(0,\ \omega_c)};$$

$$\sigma_{33}(\omega_c) = \frac{e^2\tau_3(0,\ \omega_c)}{M_3(0,\ \omega_c)}.$$

The Hall mobility μ_H is determined by the expression

$$\mu_H = c\,|\,R_H\,|\,\sigma_\perp,$$

where $R_H = E_2/hj_1 = \rho_{21}/h$ is the Hall constant. It follows from the expression for the impedance that

$$R_H = -\frac{1}{ec};\quad \mu_H = \frac{e\tau_\perp(0,\ \omega_c)}{M_\perp(0,\ \omega_c)}\,\frac{1}{1 + \omega_c^{*2}\tau_\perp^2(0,\ \omega_c)},$$

so that the Hall mobility is equal to the drift mobility $\mu(\omega_c)$ in the presence of a magnetic field in the framework of this approximation.

Optimal Choice of the Approximating Functional in Electrotransport Problems

The approximating functional $\Phi(\mathbf{r}, \mathbf{r}')$ (101) is completely determined by the impedance $Z_0(\omega)$. Indeed, it follows from the definition of the function $Z_0(\omega)$ that

$$G(\omega) = \frac{1}{2\pi}\,\frac{\mathrm{Im}\,Z_0(\omega)}{1 - e^{-\beta\omega}}.$$

On the other hand, the function $Z_0(\omega)$ can be determined from the variational principle for the free energy of the equilibrium system. Since $Z_0^{-1}(\omega)$ must be analytic for $\mathrm{Im}\,\omega > 0$, it is determined by the analytic continuation of $Z_0^{-1}(i\omega_n)$ to

the upper half-plane, which is realized by replacing $i\omega_n$ by $\omega + i\varepsilon$ [see (70a)]. In the case when a magnetic field is present it can be expected (though it has not been proved) that the inequality (13) for the free energy holds and makes it possible to determine the impedance tensor $\overleftrightarrow{Z}_0(\omega)$ of the approximating model.

Of course, there is no *a priori* guarantee that the $Z_0(\omega)$ that determines the optimal estimate of the free energy also leads to a good approximation for the impedance or the polaron conductivity. However, the more detailed discussion of this question in Refs. 118 and 119 showed that there are good arguments for assuming that the variational principle for the free energy also leads to a good approximation for the polaron impedance $Z(\omega)$. The arguments are associated with the fact that the approximate expressions (103) and (104) for the impedance satisfy a fluctuation–dissipation theorem[118] and a number of exact sum rules derived for the Pekar–Fröhlich model[118,119] if $Z_0(\omega)$ is chosen from the condition of a minimum for the free energy: $Z_0(i\omega_n) = Z(i\omega_n)$. Hence, the optimal estimate for the free energy is obtained by means of an approximating model whose impedance is equal to the polaron impedance calculated in the first approximation in accordance with the expressions (103) and (104). In other words, the approximate expression for the impedance $Z(\omega)$ is the impedance of the model $Z_0(\omega)$ for the optimal choice of the parameters.

The fluctuation–dissipation theorem relates the Fourier transform of the linear response function of the system for an external perturbation to the time correlation function associated with the given field of the dynamical quantity. In the case of the coordinate x,

$$\operatorname{Im} Z^{-1}(\omega) = \frac{1-e^{-\beta\omega}}{1+e^{-\beta\omega}} \operatorname{Re} \int_0^\infty dt\, e^{i\omega t} \langle [x(t),\ x(0)]_+ \rangle.$$

Since $Z_0(\omega)$ is the exact impedance of some quantum-statistical model, the fluctuation–dissipation theorem holds for it exactly. Therefore, the theorem is also satisfied exactly for $Z(\omega)$ if the correlation function $\langle [x(t), x(0)]_+ \rangle$ is calculated in the same approximation as the impedance.[118]

Note that such a result is also an argument in favor of the expansion (104) for the impedance, since the impedance obtained from (102) does not satisfy the fluctuation–dissipation theorem.[118]

Indeed, the self-consistency condition $\overleftrightarrow{Z}_0(\omega) = \overleftrightarrow{Z}(\omega)$ is more general than the variational principle for the free energy, being applicable even when the inequality (13) cannot be written down (for example, in the presence of a constant homogeneous static electric field). By means of the fluctuation–dissipation theorem (for the dynamical variable $\hat{\mathbf{p}}$) we can also obtain the following relation between the mean kinetic energy of the electron and the absorption coefficient[118]:

$$\left\langle \frac{\hat{\mathbf{p}}^2}{2} \right\rangle = -\frac{3}{4\pi} \int_{-\infty}^{\infty} d\omega \frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}} \operatorname{Im} \frac{\omega^2}{Z(\omega)}. \tag{110}$$

In addition, using scale transformations we can prove for the Pekar–Fröhlich Hamiltonian the identity[118]

$$\left\langle \frac{\hat{\mathbf{p}}^2}{2} \right\rangle \equiv -\frac{1}{2}\alpha \frac{\partial F(\alpha, \beta)}{\partial \alpha}. \tag{111}$$

It follows from (110) and (111) that[118]

$$F(\alpha, \beta) - F(0, \beta) = \frac{3}{\pi} \int_0^\alpha \frac{d\alpha'}{\alpha'} \int_0^\infty \frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}} \operatorname{Im} \frac{\omega^2}{Z(\omega, \alpha')} d\omega. \tag{112}$$

The expressions (110)–(112) were obtained for the first time at zero temperature in Ref. 119. It was also shown there by means of numerical calculations that the sum rule (112) is satisfied for the ground-state energy and impedance obtained by Feynman *et al.*[105] up to the numerical error. Such a result is of course an argument in favor of the FHIP approximation for the impedance.

However, as was shown in Ref. 118, the sum rule (112) is satisfied exactly for the free energy (32) and a whole family of different expressions for the impedance [including (104)]. Therefore (112) is a rather weak criterion for estimating the accuracy of an approximation for the impedance.

Alternative Method of Obtaining the Feynman–Hellwarth–Iddings–Platzman Results[134]

In the FHIP approach there are difficulties that have not so far been overcome. The first is that mathematically it is very complicated, since the nonequilibrium density matrix is used to calculate the linear response function, and this leads to the appearance of the double functional integral (96) over paths defined over an infinite time interval. However, the same problem can be solved by means of Kubo's formula in the framework of equilibrium theory, in which one can use a simpler one-dimensional integral over paths defined over the finite interval $[0, \beta]$. A second difficulty is that the transition from the expression (102) to the expression (104) is mathematically incorrect and can be justified only by physical arguments. There is in fact a certain ambiguity in the derivation in this approach of the expression for the impedance [see (118)]. Finally, a third difficulty is that the expression for the drift mobility at low temperatures differs by the factor $3/2\beta$ from the correct result. The source of this difficulty and a way of overcoming it still remain obscure.

It is known[37] that the conductivity $\sigma(\omega)$ can be obtained by means of Kubo's formula

$$\sigma(\omega) = \frac{e^2}{3\pi i} \int_{-\infty}^{\infty} \frac{dE}{E} \frac{\operatorname{Im} \tilde{g}_R(E)}{E+\omega+i\varepsilon}, \tag{113}$$

where for simplicity we consider the isotropic case in the absence of a magnetic field. Here, $\tilde{g}_R(E)$ is the Fourier transform of the two-time retarded commutator Green's function:

$$g_R(t-s) = i\theta(t-s) \langle [\hat{\mathbf{v}}_H(t),\ \hat{\mathbf{v}}_H(s)] \rangle,$$

and $\hat{\mathbf{v}}_H(t)$ is the operator of the electron velocity in the Heisenberg representation. The function $\tilde{g}_R(E)$ is analytic in the upper half-plane of the complex variable E and, therefore, can be obtained by analytic continuation from the points $i\omega_n$ $(n = 1, 2, \ldots)$. To determine $\tilde{g}_R(i\omega_n)$, we introduce the thermal Green's function[120]

$$G(\tau-\sigma) = \langle T\{\hat{\mathbf{v}}_H(\tau)\, \hat{\mathbf{v}}_H(\sigma)\} \rangle; \quad \tau,\ \sigma \in [0,\ \beta];$$

$$\tilde{G}(\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G(\tau),$$

where $\hat{\mathbf{v}}_H(\tau) = e^{\hat{H}\tau}\hat{\mathbf{v}}e^{\hat{H}\tau}$ and $T\{\hat{A}(\tau)\hat{B}(\sigma)\} = \theta(\tau-\sigma)\hat{A}(\tau) \times\hat{B}(\sigma) + \theta(\sigma-\tau)\hat{B}(\sigma)\hat{A}\tau$. It is well known that

$$\tilde{g}_R(i\omega_n) = \tilde{G}(i\omega_n) \quad n = 1, 2 \ldots,$$

so that to find $\tilde{g}_R(\omega)$ it is sufficient to calculate $\tilde{G}(\omega_n)$.

We now obtain a path-integral representation for $G(\tau-\sigma)$. We first express it in terms of operators in the interaction representation:

$$G(\tau-\sigma) = \frac{\mathrm{Tr}\{e^{-\beta\hat{H}_0}T[\hat{\mathbf{v}}(\tau)\hat{\mathbf{v}}(\sigma)\hat{\sigma}(\beta)]\}}{\mathrm{Tr}\, e^{-\beta\hat{H}}},$$

where $\hat{H}_0$, $\hat{v}(\tau)$, $\hat{\sigma}(\beta)$ are determined by Eqs. (62). We now introduce the generating functional

$$Z(\mathbf{y}) = \mathrm{Tr}\, e^{-\beta\hat{H}_0}T \times\exp\left\{-\int_0^\beta d\tau\left[\hat{H}_i(\tau) + \frac{1}{2}\hat{\mathbf{v}}^2(\tau) + i\dot{\mathbf{y}}(\tau)\cdot\hat{\mathbf{v}}(\tau)\right]\right\}.$$

It is readily verified that

$$Z(0) = \mathrm{Tr}\, e^{-\beta\hat{H}}; \quad G(\tau-\sigma) = -\frac{1}{Z(0)}\frac{\delta^2 Z(\mathbf{y})}{\delta\dot{\mathbf{y}}(\tau)\,\delta\dot{\mathbf{y}}(\sigma)}\Bigg|_{y=0}. \tag{114}$$

On the other hand, $Z(\mathbf{y})$ can be expressed in terms of an integral with respect to a Wiener measure[36]:

$$Z(\mathbf{y}) = \int_{\mathbf{x}(0)=0} D\mathbf{x}\, e^{-\frac{1}{2}\int_0^\beta d\tau\dot{\mathbf{x}}^2(\tau)} W_0(\dot{\mathbf{x}}+\dot{\mathbf{y}}),$$

where

$$W_0(\dot{\mathbf{x}}) = \mathrm{Tr}\, e^{-\beta\hat{H}_0}\, T\exp\left[-\int_0^\beta d\tau\{\hat{H}_i(\tau) + i\dot{\mathbf{x}}(\tau)\cdot\hat{\mathbf{v}}(\tau)\}\right];$$

$$W_0(\dot{\mathbf{x}}) = \Omega\delta[\mathbf{x}(\beta)-\mathbf{x}(0)]\prod_{\mathbf{k}} W_{\mathbf{k}}(\dot{\mathbf{x}})$$

and $W_{\mathbf{k}}(\dot{\mathbf{x}})$ is determined by (64a). Using (114) and (64b) and integrating by parts, we obtain

$$G(\tau-\sigma) = 3\delta(\tau-\sigma) - \langle\dot{\mathbf{x}}(\tau)\dot{\mathbf{x}}(\sigma)\rangle_S, \tag{115}$$

where $S[\mathbf{x}]$ is determined by the expression (10). It is obvious that (115) is a simpler mathematical expression than (96). The generalization of (115) to take into account the effects of anisotropy, an external magnetic field, phonon dispersion, and interaction with different branches of the phonon spectrum does not present fundamental difficulties.

To obtain the FHIP results by means of (113) and (115), we must replace $S[\mathbf{x}]$ in (115) by $S_0[\mathbf{x}]$ [see Eq. (25)]. The approximate expression for $\tilde{G}(\omega_n)$ obtained after calculation of the path integral has the form

$$\tilde{G}(\omega_n) = 3\left[1 + \frac{\omega_n^2}{Z_0(i\omega_n)}\right], \tag{116}$$

where $Z_0(i\omega_n)$ is determined by the expression obtained from the variational principle for the free energy. An approximate solution of this equation can be obtained by using the expression (70a) for $\Phi(\tau)$. Then

$$Z_0(i\omega_n) = -\omega_n^2 - \frac{2}{3}\frac{\alpha v^3}{3\sqrt{\pi}}\int_0^{\beta/2} d\tau C(\tau)(1-\cos\omega_n\tau) f^{-3/2}(\tau). \tag{117}$$

Analytic continuation of (116) and (117) to the upper half-plane gives

$$\tilde{g}_R(\omega) = 3\left[1 - \frac{\omega^2}{Z(\omega)}\right],$$

where $Z(\omega)$ is determined by (106). Using this expression in Kubo's formula (113), we obtain the FHIP result:

$$\sigma(\omega) = \frac{ie^2\omega}{Z(\omega)}. \tag{118}$$

The treatment given here is much simpler than in Ref. 105, and the expression for $\sigma(\omega)$ is obtained "automatically" without any additional assumptions. Of course, the difficulty associated with the low-temperature behavior of the drift mobility still remains. Two approximations were made in the derivation of (118). The first was in the replacement of the action $S[\mathbf{x}]$ by $S_0[\mathbf{x}]$ in the derivation of (116) from (115). The second was in the use of (117). Since the latter approximation is exact to powers of order α (for $\alpha \ll 1$), it cannot be the source of the difficulty, which is present already in the lowest order. On the other hand, one can attempt to take into account in (115) other terms in the expansion of $\langle\dot{\mathbf{x}}(\tau)\cdot\dot{\mathbf{x}}(\sigma)\rangle_S$ in powers of $(S-S_0)$:

$$\langle\dot{\mathbf{x}}(\tau)\cdot\dot{\mathbf{x}}(\sigma)\rangle_S = \langle\dot{\mathbf{x}}(\tau)\cdot\dot{\mathbf{x}}(\sigma)\rangle_{S_0} + \sum_{n-1}^{\infty}\frac{1}{n!}\frac{\langle\dot{\mathbf{x}}(\tau)\cdot\dot{\mathbf{x}}(\sigma)(S_0-S)^n\rangle_{S_0} - \langle\dot{\mathbf{x}}(\tau)\dot{\mathbf{x}}(\sigma)\rangle_{S_0}\langle(S_0-S)^n\rangle_{S_0}}{\langle e^{S_0-S}\rangle_{S_0}}. \tag{119}$$

It is easy to show that the first correction [corresponding to $n=1$ in (119)] is zero. This is simply a consequence of the fact that S_0 was determined by the variational principle for the free energy. Since $\langle S_0 - S\rangle_{S_0}$ at small α is proportional to α, one could conclude that (115) is also an exact expression up to powers of order α. However, this requires further consideration because for $\alpha \ll 1$ and $\beta \gg 1$ the quantity $\langle S_0 - S\rangle_{S_0}$ is proportional to $\alpha\beta$,[11] and the expansion could be invalid at low temperatures.

The suggestion that the expansion is invalid at low temperature agrees well with the known fact[23,41,121] that the quadratic approximation always leads to the Maxwell distribution function for the polaron momentum in a static electric field, while use of a distribution function of quasi-Maxwellian form in the solution of the stationary Boltzmann equation leads at low temperatures to the appearance of the additional factor $3/2\beta$ in the expression for the mobility.[21,22] However, for an electron interacting only with optical phonons, the only relaxation mechanism at low temperatures is the emission of optical phonons made possible by energy obtained from the electric field. This process has a strongly inelastic and anisotropic nature, and therefore the distribution function in a weak field is strongly non-Maxwellian.[122] At higher temperatures, the momentum distribution for the

polaron can be well approximated by a Maxwellian distribution, since the thermal energy of the polaron is always sufficient for the emission of phonons and, possibly, also scattering of it by the already existing thermal phonons. Therefore, for weak coupling and high temperatures ($\beta \gg 1$), the expression (118) leads to the same temperature dependence for the drift mobility as the Boltzmann equation.

7. POLARON IN A STRONG ELECTRIC FIELD

The behavior of polarons in strong electric fields is of great experimental and theoretical interest. Polaron effects in strong fields (of order 10^3 V/cm or more) are responsible for large energy losses of electrons in polar dielectrics[123,124] and lead to a number of specific nonlinear phenomena in electrotransport.[122,125–127] A satisfactory microscopic description of these situations requires the development of new methods to study kinetic phenomena with allowance for strong electron–phonon coupling, the inelasticity of the individual scatterings by optical phonons, and the strong interference between them (Refs. 39–41, 121, and 128–131).

It is well known that a Boltzmann equation is valid for the description of polarons in an electric field only in the case of weak coupling, relatively weak fields, and low frequencies. The conditions under which the Boltzmann description is invalid are strikingly illustrated by the example given in Ref. 39 of the electron energy losses in the dielectric part of a number of electronic devices (for more details, see Refs. 123 and 124). In the presence of a strong electric field (of the order of 10^6 V/cm), the energy lost by electrons over unit distance reaches values of 0.01–0.06 eV/Å. A typical value for Al_2O_3 ($\alpha \simeq 2.7$) is 0.03 eV/Å. Acoustic phonons can make a contribution of not more than 10^{-4} eV/Å, and the mechanisms of electron–hole pair production do not play a large part in such fields because the energy gap for these materials is very large ($\gtrsim 10$ eV). Since the energy of the optical phonons in these compounds is of order 0.05–0.1 eV [in Al_2O_3 there are longitudinal optical phonons with energies 0.060, 0.064, and 0.078 eV], to obtain a loss of such an order in terms of individual phonon emission events it is necessary to take a mean free path of order 3–4 Å or an electron mean free time of order 2×10^{-15} sec. If it is borne in mind that at room temperature phonon absorption is also important, it can be seen that these parameters are in fact even larger. It is clear that a consistent description of this phenomenon in the framework of the Boltzmann approximation or by means of linear response theory is impossible.

In Ref. 39, Thornber and Feynman developed a new approach to the study of polaron kinetics in a strong static electric field. Their aim was to obtain the relation $E = E(v)$ between the external field E and the velocity v achieved by the electron (it being assumed that for not too strong fields a steady state is achieved in which the electron moves with constant velocity). The approach of Ref. 39 is based on a balance equation for the total momentum of the system and uses a Galileo transformation to go over to a frame moving with the electron. The exact expressions represented in terms of path integrals are approximated by a model in which the electron interacts with a distribution of oscillators. The resulting picture is physically reasonable for all values of α, β, and E, but the authors point out two difficulties which have so far not yet been overcome.

1. The results obtained on the basis of the balance equation for the momentum do not agree with the results obtained by starting from the balance equation for the energy.

2. In the weak-field limit, the value obtained for the mobility is not equal to the mobility obtained on the basis of the Boltzmann equation (differing, as in Ref. 105, by the factor $3/2\beta$).

It was shown later[21,22] that the result of the theories of Thornber and Feynman can (only in the weak-coupling limit) be obtained from a Boltzmann equation if it is assumed that its steady solution has the form of a quasi-Maxwellian distribution. The point is that, on the one hand, the approximation of the polaron model by a quadratic functional always leads to a momentum distribution function of quasi-Maxwellian type,[23,41,121] the effective polaron temperature being independent, moreover, of the electric field intensity. At the same time, investigations of the exact solution of the Boltzmann equation (Refs. 92, 98, 99, and 131) and experimental data on measurement of the polaron drift velocity in strong electric fields at low temperatures[122,125–127] show clearly that the momentum distribution function is strongly non-Maxwellian. Qualitatively, this is due to the fact that at low temperatures and in strong fields the dominant relaxation mechanism is the emission of optical phonons, a strongly inelastic and anisotropic process which leads to a specific behavior of the charge carriers known as streaming motion. The behavior of the polarons at low temperatures in strong fields differs from the ordinary behavior of hot electrons, which can be well described by a Maxwell distribution function (with some effective temperature and mean velocity) because for them the dominant scattering mechanism (scattering by acoustic phonons and other electrons) is almost isotropic and quasielastic. At higher temperatures ($\beta \simeq 1$), a polaron can emit optical phonons by drawing on its thermal energy and it can also absorb the already existing thermal phonons, so that the nature of the relaxation mechanisms changes, the level of randomization is sufficient, and it can be expected that the situation can be more satisfactorily described by a quasi-Maxwellian distribution function.

Despite the difficulties mentioned above, the theory developed in Ref. 39 is as yet the only microscopic theory of polarons with arbitrary coupling in a strong electric field. It explains the energy losses of electrons in passing through an ionic crystal and gives a clear physical picture of the relaxation processes due to the coupling to the optical phonons. Therefore, it is of considerable interest to present this approach in more detail and discuss the essence of the approximations made in it.

The Balance-Equation Method

A polaron in a constant homogeneous field of strength E can be described by the Hamiltonian (90) with the particular choice $E(t) = Ee^{\epsilon t}$ ($t > t_0$). Suppose that as $t - t_0 \to \infty$ a steady state is attained in which the electron moves with constant velocity $\mathbf{v}$. The equation of motion for the operator

of the electron momentum

$$\frac{d}{dt}\hat{\mathbf{p}} = i\,[\hat{H},\ \hat{\mathbf{p}}]$$

leads in a steady state to the condition[39]

$$e\mathbf{E} = \sum_{\mathbf{k}} \mathbf{k} R_{\mathbf{k}}. \tag{120}$$

It describes the balance between the momentum that the electron acquires in unit time from the electric field and the momentum transmitted to the lattice through the coupling to the phonons:

$$R_{\mathbf{k}} = iQ(k)\langle \hat{a}_{\mathbf{k}}^{+} e^{-i\mathbf{k}\cdot\mathbf{r}} - \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\rangle;$$
$$\langle \ldots \rangle = \lim_{t_0 \to -\infty} \mathrm{Tr}\{\hat{\rho}(t) \ldots\}.$$

The quantity $R_{\mathbf{k}}$ depends on the parameters α, β, and E and is the difference between the number of phonons with momentum $\mathbf{k}$ emitted and absorbed in unit time in the steady state.

There is an analogous condition for the energy balance in the system. For this, one can proceed from the identity

$$\frac{d\hat{H}}{dt} \equiv i\,[\hat{H},\ \hat{H}] = 0.$$

In the steady state,

$$\frac{d}{dt}\left\langle \frac{\hat{\mathbf{p}}^2}{2} \right\rangle = i\left\langle \left[\hat{H},\ \frac{\hat{\mathbf{p}}^2}{2}\right]\right\rangle = 0;$$
$$\frac{d}{dt}\langle \hat{H}_{\mathrm{int}} \rangle = i\langle [\hat{H},\ \hat{H}_{\mathrm{int}}]\rangle = 0.$$

Then $\langle [\hat{H}_{\mathrm{ph}}, \hat{H}]\rangle + \langle [eEx, \hat{H}]\rangle = 0$, which leads to the condition

$$eEv = \sum_{\mathbf{k}} R_{\mathbf{k}};\ \ \mathbf{v} = \langle \hat{\mathbf{p}} \rangle. \tag{121}$$

Equation (121) expresses the balance between the energy that the electron acquires in unit time from the electric field and the energy transferred to the lattice by the coupling to the phonons. A path-integral representation for $R_{\mathbf{k}}$ was obtained in Ref. 39. It can be written in the form

$$R_{\mathbf{k}} = 2Q^2(k)\,\mathrm{Re}\int_0^\infty dt\, e^{-\varepsilon t}\left\{\frac{e^{-it}}{1-e^{-\beta}}\langle e^{-i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_\Phi - \frac{e^{it}}{e^{\beta}-1}\langle e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_\Phi\right\}, \tag{122}$$

where the functional Φ is determined by Eqs. (97) for $E(t) = E'(t) = Ee^{-\varepsilon t}$.

With allowance for (122), the balance conditions (120) and (121) become

$$e\mathbf{E} = 2\mathrm{Re}\sum_{\mathbf{k}} \mathbf{k}Q^2(k)\int_0^\infty dt\, e^{-\varepsilon t}\left\{\frac{e^{it}}{e^{\beta}-1} + \frac{e^{-it}}{1-e^{-\beta}}\right\} \times \langle e^{-i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_\Phi; \tag{123}$$

$$eEv = 2\,\mathrm{Re}\sum_{\mathbf{k}} Q^2(k)\int_0^\infty dt e^{\varepsilon t}\left\{\frac{e^{-it}}{1-e^{-\beta}} - \frac{e^{it}}{e^{\beta}-1}\right\} \times \langle e^{-i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_\Phi. \tag{124}$$

The expressions (123) and (124) are exact. Their generalization to the case when the crystal is anisotropic, the electron interacts with several branches of the phonon spectrum, and the system is subject to an external magnetic field and also an alternating electric field was obtained in Refs. 40, 41, and 129.

However, as we have already noted, the right-hand sides of (123) and (124) do not depend explicitly on the velocity $\mathbf{v}$. Therefore, the expression (123) does not make it possible to find the relation $E(v)$ without further assumptions making it possible to transform (at least approximately) the function $R_{\mathbf{k}}(\alpha, \beta, \mathbf{E})$ into a function of α, β, and $\mathbf{v}$. This is the essence of the approach of Ref. 39 and the approximations made there.

To obtain the results of Ref. 39, we make a substitution of the functional variables:

$$\mathbf{r}(t) = \mathbf{R}(t) + \mathbf{v}t;\quad \mathbf{r}'(t) = \mathbf{R}'(t) + \mathbf{v}t. \tag{125}$$

From (123) and (124), we obtain

$$e\mathbf{E} = 2\mathrm{Re}\sum_{\mathbf{k}} \mathbf{k}Q^2(k)\int_0^\infty dt\, e^{-\varepsilon t}\left[\frac{e^{it}}{e^{\beta}-1} + \frac{e^{-it}}{1-e^{-\beta}}\right] \times e^{-i\mathbf{k}\cdot\mathbf{v}t}\langle e^{-i\mathbf{k}\cdot[\mathbf{R}(t)-\mathbf{R}(0)]}\rangle_{\Phi'};$$

$$eEv = 2\,\mathrm{Re}\sum_{\mathbf{k}} Q^2(k)\int_0^\infty dt\, e^{-\varepsilon t}\left[\frac{e^{-it}}{1-e^{-\beta}} - \frac{e^{it}}{e^{\beta}-1}\right] \times e^{-i\mathbf{k}\cdot\mathbf{v}t}\langle e^{-i\mathbf{k}\cdot[\mathbf{R}(t)-\mathbf{R}(0)]}\rangle_{\Phi'},$$

where

$$\Phi'(\mathbf{R}, \mathbf{R}') = \int_0^\infty dt\left\{\frac{1}{2}[\dot{\mathbf{R}}^2(t) - \dot{\mathbf{R}}'^2(t)] + Ee^{-\varepsilon t}[x(t) - x'(t)]\right\} + V'(\mathbf{R}) - V'^{*}(\mathbf{R}') + U'(\mathbf{R}, \mathbf{R}');$$

$$V'(\mathbf{R}) = i\sum_{\mathbf{k}} Q^2(k)\int_0^\infty dt\int_0^t ds\, e^{-\varepsilon(t+s)} \times C[i(t-s)]\, e^{i\mathbf{k}\cdot[\mathbf{R}(t)-\mathbf{R}(s)]+i\mathbf{k}\cdot\mathbf{v}(t-s)};$$

$$U'(\mathbf{R}, \mathbf{R}') = -i\sum_{\mathbf{k}} Q^2(k)\int_0^\infty dt\int_0^\infty ds\, e^{-\varepsilon(t+s)} \times C[i(t-s)]\, e^{i\mathbf{k}[\mathbf{R}(t)-\mathbf{R}(s)]+i\mathbf{k}\cdot\mathbf{v}(t-s)}.$$

After this formal change in variables, which does not change the physical meaning or content of the expressions, the following approximations are made in Ref. 39:

a) the change of variables (125) is interpreted as a transition to a frame of reference S' moving with the electron;

b) it is assumed that for an observer in S' the correlation function $\langle \exp\{-i\mathbf{k}\cdot[\mathbf{R}(t) - \mathbf{R}(0)]\}\rangle_{\Phi'}$, which is determined by the fluctuations of the electron with respect to its mean path, is the same as for an observer in the system S in the absence of the electric field, and then

$$\langle e^{-i\mathbf{k}\cdot[\mathbf{R}(t)-\mathbf{R}(0)]}\rangle_{\Phi'} \to \langle e^{-i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_{\Phi}\big|_{E=E'=0};$$

c) the correlation function $\langle e^{-i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}\rangle_{\Phi}\big|_{E=E'=0}$ can be calculated in the quadratic approximation, i.e., by replacing the functional Φ by Φ_0 [see Eq. (101)], i.e.,

$$\langle e^{-ik\cdot[r(t)-r(0)]}\rangle_{\Phi}|_{E=E'=0} \to \langle e^{-ik\cdot[r(t)-r(0)]}\rangle_{\Phi_0}|_{E=E'=0}.$$

This last correlation function is expressed by a Gaussian integral and is calculated exactly. The result is

$$\langle e^{-ik\cdot[r(t)-r(0)]}\rangle_{\Phi_0}|_{E=E'=0} = e^{-\frac{k^2}{2}K_\beta(t)},$$

where

$$K_\beta(t)=\frac{1}{\pi i}\int_0^\infty d\omega\left(\frac{1-e^{i\omega t}}{1-e^{-\beta\omega}}+\frac{1-e^{-i\omega t}}{e^{\beta\omega}-1}\right)\left(\frac{1}{Z_0^*(\omega)}-\frac{1}{Z_0(\omega)}\right)$$

and $Z_0(\omega)$ is determined by (103). In the special case of Feynman's single-oscillator model, the function $K_\beta(t)$ is given by

$$K_\beta(t)=\frac{1}{v^2}\left\{\frac{\beta}{4}+\frac{t^2}{\beta}+\frac{v^2-1}{Wv}\frac{\operatorname{ch}\frac{\beta Wv}{2}-\cos Wvt}{\operatorname{sh}\frac{\beta Wv}{2}}\right\}.$$

After these approximations, the expressions (123) and (124) in the limit $\varepsilon \to 0$ take the final form

$$e\mathbf{E}=\sum_{\mathbf{k}}\mathbf{k}Q^2(k)\int_{-\infty}^{\infty}dt\,C(it)\,e^{-ik\cdot vt-\frac{k^2}{2}K_\beta(t)}; \qquad (126)$$

$$eEv=\sum_{\mathbf{k}}Q^2(k)\int_{-\infty}^{\infty}dt\,e^{-ik\cdot vt-\frac{k^2}{2}K_\beta(t)}\left[\frac{e^{-it}}{1-e^{-\beta}}-\frac{e^{it}}{e^{\beta}-1}\right]. \qquad (127)$$

Thus, in the framework of the approximations of Ref. 39 the only effect of the external electric field is that under its influence the electron acquires a certain mean velocity $\mathbf{v}$ but there is no effect on the fluctuations of the electron about its mean path. Therefore, the effective electron temperature does not depend on the field strength.

As we have already said, the expression (126) in the weak-field limit leads to the expression (89) for the drift mobility. Another difficulty of this approach is that the expressions (126) and (127) are not equivalent, leading to the same results only if $K_\beta(t)$ does not depend on t. Feynman and Thornber[39] prefer the expression (126) because it is physically reasonable for all values of the parameters α, β, and E, whereas (127) leads to an expression for the drift mobility according to which mobility increases with the temperature. Thus, the approximate solution of the polaron problem in an electric field obtained in Ref. 39 does not guarantee energy conservation in the system.

We note also that the transition to the frame S' through the change of variables (125) differs from the method used in Sec. 3 to determine the effective polaron mass. The approximation of Ref. 39 does not take into account the Doppler shift of the phonon frequencies for an observer moving with velocity $\mathbf{v}$. However, the procedure used in Sec. 3 is restricted to the case of infinitesimally small velocities and needs to be generalized when it is applied to a problem in which the electron moves with finite velocity.

Behavior of Polarons in an Electric Field

In Ref. 39, on the basis of (126) and numerical calculations, Feynman and Thornber obtained a family of curves $E(\mathbf{v})$ for $\alpha = 3, 5, 7$ and $\beta = 20, 10, 5, 1, 0.1, 0.01, 0.001$; this family makes it possible to study the complete physical picture of the polaron energy loss in a strong field. All the results can be interpreted in terms of the competition between the mechanisms of absorption and emission of optical phonons by a polaron of mass $m_0^* = v^2$.

The main features of their picture are as follows.

a) The energy losses $eE(v)$ over unit distance increase with v and reach a maximum eE_1 at a certain threshold velocity $v_1(\alpha,\beta)$. For $E > E_1$, the electron–phonon coupling can no longer restrain the electron, which is accelerated without limit under the influence of the electric field. Of course, in a real crystal there come into play other energy-loss mechanisms that are not taken into account in the Pekar–Fröhlich Hamiltonian and which determine the relaxation in such fields (for example, interband transitions). For $v > v_1$, the derivative is $dE/dv < 0$, and this corresponds to an unstable regime in which v ceases to have the physical meaning of a steady velocity. The losses at fixed velocity increase monotonically with the temperature and with the coupling parameter α.

b) At low temperatures ($\beta \gg 1$), the velocity v_1 is approximately equal to the velocity v_0 needed for the emission of an optical phonon: $\frac{1}{2}m_0^*v_0^2 = \hbar\omega_0$ ($v_0 = \sqrt{2/v}$ in our system of units). This is a consequence of the fact that for $v \lesssim v_1$ and $\beta \gg 1$ the dominant relaxation mechanism is the emission of optical phonons. With increasing α, the velocity v_1 decreases because of the increase in the effective polaron mass. With increasing temperature, v_1 increases and differs appreciably from v_0 (for $\beta < 1$, $v_1 > \sqrt{2} > v_0$) because scattering by thermal phonons begins to play an important part.

c) For $v < v_1$, there are two regimes—a linear regime in which the relaxation is determined by scattering by thermal phonons at low velocities, and a nonlinear, almost temperature-independent regime in which the losses are determined by the emission of optical phonons at higher velocities. If $\beta > 2$, the polaron goes over very rapidly to this nonlinear regime, which is characterized by the rapid acquisition of energy from the electric field and its loss by phonon emission.

The maximal energy losses for Al_2O_3 were also estimated in Ref. 39. Feynman and Thornber took the values $\hbar\omega_0 = 0.07$ eV, $\varepsilon_\infty = 3.1$, $\varepsilon_0 = 9.0$, and $m = m_e$; then $\alpha = 2.7$, and at low temperatures $eE_1 = 0.025$ eV/Å, in good agreement with the experimental value of 0.03 eV/Å.[123]

In Ref. 121, Peeters and Devreese developed an alternative method of obtaining the results of Ref. 39 by using the equation of motion for the operators in the Heisenberg representation, and they showed explicitly that the momentum distribution function in the approximation of Ref. 39 has the form

$$f(\mathbf{p})=\left(\frac{\beta_e}{2\pi}\right)^{3/2}\exp\left\{-\frac{\beta_e}{2}(\mathbf{p}-\mathbf{v})^2\right\},$$

where β_e, the effective reciprocal temperature, depends on α and β and is given by

$$\beta_e=\beta v^2\left\{1+(v^2-1)\frac{\beta Wv}{2}\operatorname{cth}\frac{\beta Wv}{2}\right\}^{-1}.$$

Note that $\beta/\beta_e \to 0$ as $\beta \to \infty$ if $v \neq 1$. This means that at

low temperatures the effective temperature differs strongly from the lattice temperature even in the case of weak coupling.

Analysis of the experimental data on the mobility in AgBr and AgCl at $T = 4.2$ °K and in strong fields shows that the limiting polaron velocity is $v_1 < 3\sqrt{2}/4 \simeq 1.06$.[122] The results of Ref. 39 give $v_1 \simeq v_0 = \sqrt{2}/v = 1.23$ for AgBr($\alpha = 1.6$). A comparison was made in Ref. 121, in which the discrepancy was attributed to the fact that the nonparabolicity of the polaron dispersion law leads to an increase in the effective mass with the velocity and that to take into account this effect it is necessary to make allowance for the dependence of the variational parameters v and W on the velocity. We note that this can be done on the basis of the inequality (70) for $\beta = \infty$.

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