

Temperature dependence of the polaron*

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We point out that the existing literature is not even clear on which direction the polaron energy should change with temperature. We analyze the existing simple calculations and show that they are most easily understood in terms of phonon-frequency shifts, rather than a temperature-dependent polaron self-energy. We show further that there are two different ways of defining a temperature-dependent polaron energy level, both of which play a role in some calculations. We use a temperature-dependent form of the intermediate-coupling theory which gives results that are qualitatively acceptable.

I. INTRODUCTION

The literature on the temperature dependence of the polaron is in a state of confusion. Two contradictory strains have existed for years with essentially no interaction. There is a series of papers that claim that as temperature increases the polaron loses its phonon clothing and becomes free-electron-like. There is another series of papers that claim, to the contrary, that as the temperature increases the polaron becomes more deeply bound and its effective mass increases.

Probably the earliest serious consideration of the temperature dependence of the polaron energy was the work of Yokota,¹ who obtained for the optical polaron the energy-momentum relation

$$\epsilon(k) = \frac{-\alpha}{(2\bar{n}^0 + 1)^{1/2}} + \frac{k^2}{[1 + \alpha/6(2\bar{n}^0 + 1)^{3/2}]}. \quad (1)$$

We have chosen units so that $\hbar = 2m = \omega = 1$. The coupling constant is α and

$$\bar{n}^0 = 1/(\epsilon^\beta - 1),$$

where $\beta = (k_B T)^{-1}$. The calculation is a temperature-dependent version of the $T = 0^\circ \text{K}$ intermediate-coupling theory which was done by Yokota² as well as by Lee, Low, Pines³ and by Gurari.⁴ Figure 1 shows, qualitatively, how this energy varies with temperature. At $T = 0^\circ \text{K}$ we have the usual intermediate-coupling theory. As T increases, the self-energy disappears and the effective mass approaches that of a free electron (i. e., no electron-phonon interaction). This type of temperature dependence, at first thought, seems quite reasonable. The polaron, which is a sort of bound state, ionizes like any other bound system does as temperature increases. This same result has been obtained from another version of the intermediate-coupling theory by Porsch⁵ and, independently, by the present authors.⁶ Osaka⁷ and Krivoglaz and

Pekar⁸ have obtained the same qualitative result from a different point of view using the Feynman theory. The same qualitative conclusion has been obtained for the piezoelectric polaron from two different approaches by Okamoto⁹ and Porsch.¹⁰

On the other hand, Fulton¹¹ has used a different extension of the intermediate-coupling theory to $T \neq 0^\circ \text{K}$ and obtained instead of Eq. (1)

$$\epsilon(k) = -(\bar{n}^0 + 1)\alpha + k^2 [1 - \frac{1}{6}(\bar{n}^0 + 1)\alpha]. \quad (2)$$

Figure 2 shows how this energy varies with temperature. Again we get the usual intermediate-coupling theory at $T = 0^\circ \text{K}$, but as T increases the self-energy increases (i. e., becomes more negative) and the effective mass increases. In short, the polaron effects become larger, which is at first thought surprising, for the same reason that Eq. (1) seemed reasonable. Equation (2) is also obtained both from simple perturbation theory (as we will discuss below) and from the lowest-order temperature-dependent Green's-function approximations, either perturbation theory¹² or Tamm-Dancoff.¹²

In the cases where the electron interacts with acoustic phonons the phonon frequency is wave-vector dependent, and hence the phonon distribution function \bar{n}^0 can no longer be pulled out of the integrals over wave vector. Nevertheless, the same dichotomy exists between theories that give increasing and decreasing temperature-dependent energies. Mahan and Hopfield¹³ and Osaka¹⁴ have analyzed the piezoelectric polaron using perturbation theory and Tamm-Dancoff, respectively, and have obtained results that vary like Eq. (2). In analyzing the temperature dependence of the band gap in semiconductors Fan¹⁵ and others^{16,17} have again used perturbation theory to get a temperature dependence like Eq. (2). In both of these works, which are concerned with acoustic phonons, there is the additional point that \bar{n}^0 can become

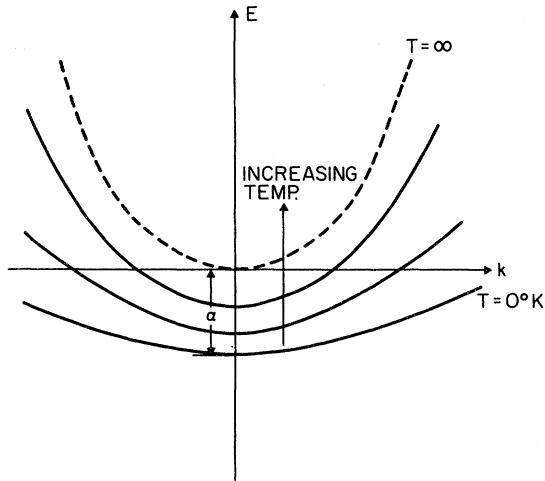


FIG. 1. Temperature dependence of the polaron energy-momentum relation according to Eq. (1). This is the type of temperature dependence that we would expect.

large at reasonable temperatures. Hence, the temperature-dependent part of the shift is much larger than the temperature-independent part. For instance between 4 and 400°K the experimentally measured band gap of germanium shifts by about 10^{-3} eV, which is an order of magnitude larger than the zero-temperature polaron self-energy. The sign of this energy shift requires that the electron be more deeply bound at higher temperatures. However, it is difficult to see this effect as being due to the polaron self-energy. On the other hand, two other works on acoustic phonons^{9,10} give just the opposite temperature dependence.

The contradiction between the results of Fulton and Yokota was recognized by Schultz¹⁸ and Osaka.⁷ Both comment (as does Fulton) that Fulton's results are based on varying an excited state that is not orthogonal to exact lower states, and hence his results are of questionable validity. However they do not resolve the situation completely, particularly since the lowest-order perturbation theory gives qualitatively the same results, and they are widely¹³⁻¹⁷ accepted.

Krivoglaz and Pekar⁸ have approached the problem in a different way. Instead of trying to define temperature-dependent energy levels they calculate the total partition function both in perturbation theory and in the Feynman theory. From their results one cannot infer what temperature-dependent energy level could or should be used. However a perturbation approach to the temperature-dependent energy levels can be used to get their perturbation results. We are more interested in the temperature-dependent energy levels because we hope that they will be useful in interpreting a wide va-

riety of experimental results.

Since the simplest and most direct way of getting results like Eq. (2) is by perturbation theory, we will examine this approach in detail in Sec. II. We will show that the results are easily understood if we realize that they are caused by the phonon re-normalization, not the electron self-energy. With this realization in mind we can easily do an improved calculation which completely reverses the character of the results.

In Sec. II we start with the second-order perturbation-theory energy levels and calculate the partition function without further approximation. We can then see that two different temperature-dependent energy levels both play a role. One we call a temperature-dependent free energy level because it gives the probability of the state being occupied. The other we call a temperature-dependent internal energy level because it gives the contribution that the state makes to the internal energy. The internal energy level has a temperature dependence like Eq. (1) and the free energy level has a temperature dependence like Eq. (2). Hence both types have some validity.

In Sec. III we do a calculation based on the intermediate-coupling theory which permits an intrinsic temperature dependence of the electron self-energy, as well as including the effects which dominate the perturbation-theory discussion. The results of this theory are quite different from the version based on perturbation theory, and we feel that they are at least qualitatively acceptable.

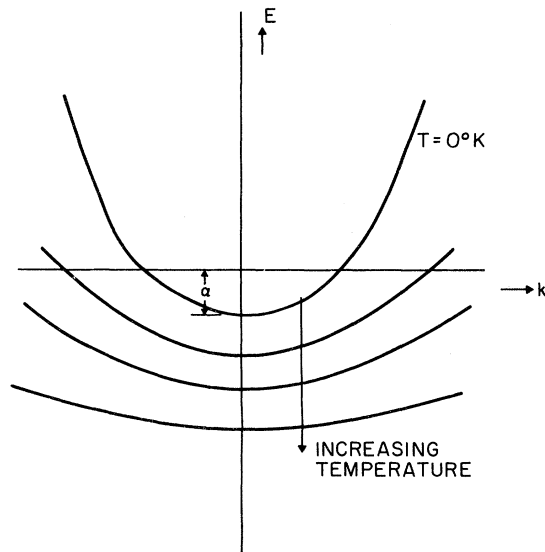


FIG. 2. Temperature dependence of the polaron energy-momentum relation according to Eq. (2), and perturbation theory.

II. PERTURBATION THEORY

A. Electron and phonon self-energy

First we will analyze the most straightforward, naïve (and also the most commonly used) way of obtaining the temperature dependence of the polaron. We start with the usual Fröhlich Hamiltonian, written in dimensionless units,

$$H = H_0 + H_{\text{int}},$$

$$H_0 = p^2 + \sum_q (a_q^\dagger a_q + \frac{1}{2}) \omega(q),$$

$$H_{\text{int}} = \sum_q Q(q) (a_{-q}^\dagger + a_q) e^{i\vec{q}\cdot\vec{r}}.$$

Table I shows the values of $\omega(q)$, $Q(q)$ and the units used for the different types of phonons involved. In the table m , ω , and s are the band effective mass of the carrier, the optical-phonon frequency, and the speed of sound. The values of these constants as also the values of $\alpha_1 \rightarrow \alpha_4$ depend on the crystal. Henceforth we shall drop the subscripts on the α 's and refer to the dimensionless coupling constant as α .

Let us use second-order perturbation theory to calculate the shift in the energy of the state

$$|i\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{v}} \prod_q (a_q^\dagger)^{n(q)} / \left(\prod_q n(q)! \right)^{1/2} |0\rangle,$$

which is an eigenstate of H_0 with eigenvalue

$$E_i = k^2 + \sum_q [n(q) + \frac{1}{2}] \omega(q).$$

The shifted energy is

$$E(\vec{k}, \{n(q)\}) = E_i + \sum_{f \neq i} \frac{|\langle f | H_{\text{int}} | i \rangle|^2}{E_i - E_f},$$

which becomes

$$E(k, \{n(q)\}) = E_i + \sum_q Q^2(q) \left(\frac{n(q) + 1}{2\vec{k} \cdot \vec{q} - q^2 - \omega(q)} + \frac{n(q)}{-2\vec{k} \cdot \vec{q} - q^2 + \omega(q)} \right).$$

TABLE I. Values of $\omega(q)$, $Q(q)$ and units used for different types of phonons.

Type of interaction	$\omega(q)$	$Q(q)$	Unit of energy	Unit of length
Polar, optical	1	$\left(\frac{4\pi\alpha_1}{V}\right)^{1/2} \frac{1}{q}$	$\hbar\omega$	$\left(\frac{\hbar}{2m\omega}\right)^{1/2}$
Piezoelectric, acoustic	q	$\left(\frac{4\pi\alpha_2}{V}\right)^{1/2} \frac{1}{\sqrt{q}}$	$2ms^2$	$\frac{\hbar}{2ms}$
Deformation potential acoustic	q	$\left(\frac{4\pi\alpha_3}{V}\right)^{1/2} \frac{1}{\sqrt{q}}$	$2ms^2$	$\frac{\hbar}{2ms}$
Deformation potential optical	1	$\left(\frac{4\pi\alpha_4}{V}\right)^{1/2}$	$\hbar\omega$	$\left(\frac{\hbar}{2m\omega}\right)^{1/2}$

For reasons that will become clear below, we will break this expression into parts that are associated with the electron and phonon energies, respectively. We write

$$E(k, \{n(q)\}) = k^2 - \delta\epsilon(\vec{k}) + \sum_q [n(q) + \frac{1}{2}] [\omega(q) - \delta\omega], \quad (3)$$

where

$$\delta\epsilon(k) = - \sum_q \frac{1}{2} Q^2(q) \left(\frac{1}{k^2 - (k-q)^2 - \omega(q)} - \frac{1}{k^2 - (k+q)^2 + \omega(q)} \right),$$

$$\delta\omega(q, k) = - Q^2(q) \left(\frac{1}{k^2 - (k-q)^2 - \omega(q)} + \frac{1}{k^2 - (k+q)^2 + \omega(q)} \right). \quad (4)$$

This sort of separation of the correction is common in the theory of metals,¹⁹ but not in insulators and semiconductors. The usual procedure at this point is to replace the phonon occupation numbers by their thermal equilibrium expected values

$$\bar{n}^0(q) \equiv (e^{+\beta\omega(q)} - 1)^{-1}, \quad (5)$$

and hence obtain a temperature-dependent version of the theory

$$E(k, \{n(q)\}) \rightarrow E_1(k, T) = k^2 - \delta\epsilon(k) + \sum_q (\bar{n}^0 + \frac{1}{2}) [\omega(q) - \delta\omega]. \quad (6)$$

This procedure can be justified by more careful arguments which we will consider in detail Sec. II B, but first we would like to make several observations about the result:

(i) $\delta\epsilon(\vec{k})$ can be thought of as the electron self-energy and $\delta\omega$ as a shift in the phonon frequency caused by the presence of the electron. $\delta\omega \propto 1/V$ and hence is smaller than $\delta\epsilon(k)$ and ω_q by a factor of the order of 10^{-23} , but $\delta\epsilon(k)$ and $\sum_q \frac{1}{2} \delta\omega$ are of the same order of magnitude.

(ii) Note that in $E_1(k, T)$ the temperature dependence is caused entirely by the factor \bar{n}^0 , and that both $\delta\epsilon$ and $\delta\omega$ are temperature independent. Hence in this simple theory there is no tendency for the polaron to ionize as temperature increases. The entire temperature dependence may be viewed as due to the effect that interaction with the electron has on the phonon frequencies. The shift in frequency can be either positive or negative depending on the values of \vec{k} and \vec{q} , but, the net shift in the energy of all the phonons, given by $-\sum_q \delta\omega_{q,k}$ is negative. As the temperature increases more phonons appear, and the interacting system has an increasingly lower energy than the noninteracting system. This effect accounts for all of the temper-

ature dependence which we found hard to understand in Sec. I. We regard the fact that the polaron shows no tendency to ionize as a weakness of this theory, a weakness which will be corrected in Sec. III where we discuss the intermediate-coupling theory.

(iii) However, even if we stay within the context of theories with temperature-independent $\delta\epsilon$ and $\delta\omega$, there is another serious weakness in the procedure that leads to $E_1(k, T)$. Once we recognize that the temperature dependence that we are seeing comes from a shift of the phonon frequencies rather than the electron energy it is natural to suggest that, instead of replacing $n(q)$ by $\bar{n}^0(q)$, we should replace it by

$$\bar{n}(q) \equiv (e^{+\beta(\omega - \delta\omega)} - 1)^{-1}, \quad (7)$$

thus obtaining

$$E(k, \{n(q)\}) \rightarrow E(k, T) = k^2 - \delta\epsilon(k) + \sum_q [\bar{n}(q) + \frac{1}{2}] (\omega - \delta\omega). \quad (8)$$

We must not make the error of dropping the $\delta\omega$ in \bar{n} even though it is much smaller than ω . Instead let us expand \bar{n} in powers of $\delta\omega/\omega$ and keep only the lowest term. We get

$$E_2(k, T) = E_1(k, T) + \sum_q \bar{n}^0(\bar{n}^0 + 1) \omega \beta \delta\omega. \quad (9)$$

The origins of the two temperature-dependent terms in Eq. (9) are clear. The temperature dependence of $E_1(k, T)$ comes from

$$-\sum_q \bar{n}^0 \delta\omega.$$

But, if the phonon frequencies are lowered, the phonon occupation numbers will increase, giving rise to the second positive term in Eq. (9). At high temperature

$$\sum_q \bar{n}^0(\bar{n}^0 + 1) \omega \beta \delta\omega \approx \sum_q \bar{n}^0 \delta\omega,$$

and the leading temperature dependence in $E_1(k, T)$ is just cancelled.

At low temperatures the positive term dominates and the temperature dependence of $E_2(k, T)$ is just opposite to that of $E_1(k, T)$. Hence, a more plausible form of the usual naïve argument [Eq. (6)] leads to the opposite kind of temperature dependence (i. e., the energy goes up with temperature). We will show in Sec. IIB, that even though intuition leads us to E_2 rather than E_1 , when we are more careful we find that E_1 also plays a role.

B. Calculation of partition function and internal energy

In order to see clearly the role played by temperature-dependent energy levels like $E_1(k, T)$ and $E_2(k, T)$ we will start from the temperature-inde-

pendent energy levels $E(k, \{n(q)\})$ given in Eq. (6) and derive expressions for the partition function and internal energy that involve temperature-dependent energy levels. Since $E(\vec{k}, \{\bar{n}(\vec{q})\})$ is so simple and $\delta\omega/\omega$ so small this can be done essentially without approximation [except, of course, the approximation involved in using $E(\vec{k}, \{n(\vec{q})\})$].

The partition function is given by

$$Z = \sum_{\vec{k}, \{n(\vec{q})\}} e^{-\beta E(k, \{n(\vec{q})\})}, \quad (10)$$

$$= \sum_{\vec{k}} e^{-\beta \epsilon(\vec{k})} \prod_{n(\vec{q})=0}^{\infty} \exp\left(-\beta \sum_q n(\vec{q}) (\omega - \delta\omega)\right), \quad (11)$$

where

$$\epsilon(\vec{k}) = k^2 - \delta\epsilon - \sum_q \frac{\delta\omega - \omega}{2}. \quad (12)$$

After doing the sums on $\{n(\vec{q})\}$, we have

$$Z = \sum_{\vec{k}} e^{-\beta \epsilon(\vec{k})} \prod_q \frac{1}{1 - e^{-\beta\omega}} \prod_q \frac{1}{1 - \bar{n}^0 (e^{\beta\delta\omega} - 1)}. \quad (13)$$

Remembering that $\delta\omega/\omega \sim 10^{-23}$ we can write

$$\begin{aligned} \prod_q \frac{1}{1 - \bar{n}^0 (e^{\beta\delta\omega} - 1)} &= \prod_q \frac{1}{1 - \bar{n}^0 \beta \delta\omega} + O\left(\frac{1}{N}\right) \\ &= \exp\left(\sum_q \bar{n}^0 \beta \delta\omega\right) + O\left(\frac{1}{N}\right). \end{aligned} \quad (14)$$

These equations can most easily be verified by taking the logarithms of both sides and expanding.

The partition function then becomes

$$Z = \sum_{\vec{k}} \exp\left[-\beta\left(\epsilon(k) - \sum_q \bar{n}^0 \beta \delta\omega\right)\right] \prod_q \frac{1}{1 - e^{-\beta\omega}}. \quad (15)$$

The internal energy

$$\bar{E} = -\frac{\partial}{\partial \beta} \ln Z, \quad (16)$$

can be written

$$\bar{E} = \sum_{\vec{k}} e^{-\beta E_1(k, T)} E_2(k, T) / \sum_{\vec{k}} e^{-\beta E_1(k, T)} + \sum_q \bar{n}^0 \omega_q. \quad (17)$$

We see that both E_1 and E_2 play a role in determining \bar{E} . The energy E_1 which appears in the exponent determines the probability that the effective state is occupied. Hence it should be thought of as a "free energy level." The energy E_2 gives the contribution to \bar{E} that is made by that state if it is occupied, and should be thought of as a temperature-dependent "internal energy level." This distinction was realized years ago by James²⁰ and Elcock and Landsberg.²¹ But it was applied only to temperature dependence of band gaps in semi-

conductors, and it was not clear from this example that the two types of temperature-dependent energy levels moved in *opposite* directions as the temperature changed. Moreover the relevance of this early work to the polaron problem has not been appreciated.

Although the effects we have been describing are quite real, this description has been based on the lowest-order perturbation-theory energy levels. This description does not permit any inherent temperature dependence in the polaron self-energy or the phonon frequency renormalization (i. e., the tendency for the polaron to ionize as temperature increases has been entirely neglected). In what follows we show how a more complete calculation can remedy this defect.

III. INTERMEDIATE-COUPLING THEORY

In the intermediate-coupling theory²⁻⁴ the noninteracting eigenstates are transformed to

$$e^{-S_1} \exp \left[i \left(\vec{P} - \sum_q n(q) \vec{q} \right) \cdot \vec{r} \right] \prod_q \left[\frac{(a_q^\dagger)^{n(q)}}{\left(\prod_q n(q)! \right)^{1/2}} \right] |0\rangle = e^{i\vec{P} \cdot \vec{r}} \prod_q \left[\frac{(a_q^\dagger)^{n(q)}}{\left(\prod_q n(q)! \right)^{1/2}} \right] |0\rangle. \quad (19)$$

We now have a new set of complete, orthonormal states which can be used to estimate the partition function. We will use these in connection with the variational principle of Peierls²² which asserts that

$$Z \equiv \text{Tr} e^{-\beta H} \geq \sum_n e^{-\beta \langle n | H | n \rangle},$$

$$\begin{aligned} E_I(P, \{n(q)\}) \equiv \langle P, \{n(q)\} | H | P, \{n(q)\} \rangle &= \left(\vec{P} - \sum_q \vec{q} n(q) \right)^2 + 2 \sum_q Q(q) f_q + \sum_q f_q^2 [\omega(q) - 2\vec{P} \cdot \vec{q} + q^2] \\ &+ \left(\sum_q \vec{q} f_q^2 \right)^2 + \sum_q n(q) \left(\omega(q) + 2\vec{q} \cdot \sum_{q'} \vec{q}' f_{q'}^2 \right) + 2 \sum_q f_q^2 q^2 n(q) + \sum_q \frac{1}{2} \omega(q). \end{aligned}$$

We now follow Yokota¹ and calculate the partition function for the polaron by fixing its momentum to be \vec{K} . Then

$$Z_K = \sum_{P, \{n(q)\}} e^{-\beta E_I(P, \{n(q)\})} \delta \left(\vec{P} - \sum_q \vec{q} n(q) - \vec{K} \right), \quad (20)$$

and the total partition function is

$$\begin{aligned} Z &= \sum_k Z_K, \\ Z_K &= \sum_{\{n(q)\}} \exp \left\{ -\beta \left[K^2 + 2 \sum_q Q_q f_q + \sum_q f_q^2 [\omega(q) - 2\vec{K} \cdot \vec{q} + q^2] + \left(\sum_q q f_q^2 \right)^2 + \sum_q \frac{1}{2} \omega(q) + \sum_q n(q) [\omega(q) + 2f_q^2 q^2] \right] \right\}. \end{aligned}$$

Performing the sums on the $\{n(q)\}$

$$Z_K = \exp -\beta \left[K^2 + 2 \sum_q Q_q f_q + \sum_q f_q^2 [\omega(q) - 2\vec{K} \cdot \vec{q} + q^2] + \left(\sum_q q f_q^2 \right)^2 + \sum_q \frac{\omega(q)}{2} \right] \prod_q \frac{1}{1 - e^{-\beta [\omega(q) + 2q^2 f_q^2]}}. \quad (21)$$

Now we vary f_q to maximize $\ln Z_K$ which amounts to minimizing the free energy, obtaining

$$\begin{aligned} |P, \{n(q)\}\rangle &= e^{S_1} e^{S_2} e^{-S_1} \exp \left[i \left(\vec{P} - \sum_q n(q) \vec{q} \right) \cdot \vec{r} \right] \\ &\times \prod_q \frac{(a_q^\dagger)^{n(q)}}{\left(n(q)! \right)^{1/2}} |0\rangle, \end{aligned} \quad (18)$$

where

$$S_1 = -i \sum_q a_q^\dagger a_q \vec{q} \cdot \vec{r}$$

and

$$S_2 = -\sum_q f_q (a_q - a_q^\dagger).$$

The total momentum of the system is P . Note that

$$e^{S_1} e^{S_2} e^{-S_1} = \exp \left(-\sum_q f_q (a_q e^{i\vec{q} \cdot \vec{r}} - a_q^\dagger e^{-i\vec{q} \cdot \vec{r}}) \right)$$

is just a displaced oscillator transformation with displacement centered on the electron. Since

$$e^{S_1} |0\rangle = |0\rangle,$$

we can write

where $|n\rangle$ stands for any orthogonal set of states. When $|n\rangle$ are energy eigenstates the equality holds.

We vary the states given by Eq. (18) with respect to the parameters f_q to get the best partition function (minimum free energy). For the energy levels we obtain

$$\begin{aligned}\tilde{f}_q &= -Q_q \left/ \left[\omega(q) - 2\tilde{q} \cdot \left(\vec{K} - \sum_{q'} \tilde{q}' f'^2(q') \right) + q^2 [1 + 2\bar{n}(q)] \right] \right., \\ \bar{n}(q) &= (e^{\beta[\omega(q) + 2q^2 \tilde{f}_q^2]} - 1)^{-1}.\end{aligned}\quad (22)$$

As is usual in the intermediate-coupling theory we define the polaron velocity by

$$\vec{K} - \sum_q \tilde{q} f_q^2 \equiv \vec{V}(\vec{K})$$

and find that $\vec{V}(\vec{K})$ satisfies the transcendental equation

$$\vec{V}(\vec{K}) = \vec{K} - \sum_q \frac{\tilde{q} Q^2(q)}{[\omega(q) - \tilde{q} \cdot \vec{V}(\vec{K}) + q^2 [1 + 2\bar{n}(q)]]^2}. \quad (23)$$

The value of the partition function Z is then easily written

$$\begin{aligned}Z_K &= e^{-\beta E(K)} \prod_q (1 - e^{-\beta[\omega(q) + 2q^2 \tilde{f}_q^2]})^{-1}, \\ E(K) &= K^2 - (V - K)^2 + 2 \sum_q Q_q \tilde{f}_q + \sum_q \frac{\omega(q)}{2} \\ &\quad + \sum_q \tilde{f}_q^2 (\omega - 2\tilde{q} \cdot \vec{V} + q^2).\end{aligned}\quad (24)$$

Once again as in Sec. II the shift in phonon frequency is small ($\sim 10^{-23}$). But in contrast to the second-order calculation the shift is positive for all wave vectors and is inherently temperature dependent. So, essentially without approximation, we can set

$$(1 - e^{-\beta[\omega(q) + 2q^2 \tilde{f}_q^2]})^{-1} = (1 - e^{-\beta\omega(q)})^{-1} e^{-\beta\pi^0 2q^2 \tilde{f}_q^2},$$

and show that the polaron partition function Z_K reduces to a product of a temperature-dependent polaron part and a free phonon part

$$\begin{aligned}Z_K &= e^{-\beta \bar{E}(K)} \prod_q (1 - e^{-\beta\omega(q)})^{-1}, \\ \bar{E}(K) &= K^2 - (K - V)^2 + \sum_q Q_q \tilde{f}_q + \sum_q \frac{\omega(q)}{2},\end{aligned}\quad (25)$$

$$Z = \sum_K Z_K.$$

Finally we calculate that the internal energy for our partition function is

$$\bar{E} = \sum_K e^{-\beta \bar{E}(K)} \left(\bar{E}(K) + \beta \frac{\partial \bar{E}(K)}{\partial \beta} \right) / Z + \sum_q \bar{n}^0 \omega(q). \quad (26)$$

It is clear from the preceding development that the LLP theory with renormalized phonons meets the requirements for a qualitatively correct temperature-dependent polaron theory. The polaron clothing is naturally temperature dependent as is the phonon frequency renormalization. The temperature dependence is such that, in both cases, the polaron reduces at high temperatures to a free electron and unrenormalized phonons. The temperature-dependent energies $\bar{E}(K)$ and $(\bar{E} + \beta \partial \bar{E} / \partial \beta)$ are the free energy and internal energy levels of the polaron of momentum \vec{K} .

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