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Temperature dependence of the polaron mass in AgBr

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The temperature dependence of the polaron mass is studied using the Feynman polaron model. The polaron mass is defined from the polaron velocity response function and corresponds to the cyclotron resonance mass in the limit of zero magnetic field. Qualitative agreement is obtained with experimental results on the temperature dependence of the cyclotron effective mass in AgBr.

There is a renewed interest[1–8] in the temperature dependence of the properties of polarons. In the past[9] most work on polarons was devoted to the calculation of the ground-state energy and the effective mass of polarons at zero temperature. Exact results are available for these properties in the limit of small and large electron-phonon coupling strength (see, e.g., Refs. 7 and 9). The Feynman polaron theory[10] provides an excellent interpolation between the small and large electron-phonon coupling regions. In contrast with the electron-phonon coupling dependence of the polaron at zero temperature, which is well-known, the behavior of the polaron mass as a function of the temperature is still a subject of discussion. Different definitions for the polaron mass and different approximations lead to significantly different dependences of the polaron mass on temperature. For sufficiently low lattice temperature some theories[5,6,8,11] predict a polaron mass that increases with increasing temperature, while other theories[2–4,7] lead to a polaron mass that decreases with increasing temperature.

The effective mass of the charge carriers in a crystal is usually determined by a cyclotron resonance experiment. Existing cyclotron resonance data at low magnetic fields in, e.g., the silver halides[12–16] show that the polaron mass increases with lattice or carrier temperature. This experimental fact is in disagreement with the temperature behavior of the polaron mass as predicted by Refs. 2–4 and 7. The purpose of the present paper is to clarify this discrepancy. It turns out that a calculation that relies on a definition of the polaron mass which is more closely connected to the experimental measured quantity is necessary.

In a recent paper[17] we calculated the cyclotron resonance absorption spectrum of polarons using the generalized Feynman polaron model and obtained

$$\mathrm{Re}\left[\frac{i}{\omega-\omega_c-\Sigma(\omega)}\right] , \tag{1}$$

with $\omega_c = eB/m_b c$ the cyclotron frequency for a band electron with mass m_b, and $\Sigma(\omega)$ is the memory function that is derived in Ref. 17. The cyclotron resonance peak occurs at a frequency $\omega=\omega_c^*$ for which $\omega-\omega_c-\mathrm{Re}\Sigma(\omega)=0$. The cyclotron mass is then defined by $m^*/m_b=\omega_c/\omega_c^*$. The magnetic field dependence of the polaron mass at zero temperature defined in this way was discussed in Ref. 17. In the present paper we are interested in the zero magnetic field limit, but we will allow temperature to be nonzero. In the limit of vanishing magnetic field the above definition of the polaron mass leads to

$$\frac{m^*}{m_b} = 1 - \lim_{\omega\to 0} \mathrm{Re}\frac{\Sigma(\omega)}{\omega} , \tag{2}$$

where the memory function $\Sigma(\omega)$ reduces to the memory function of the Feynman-Hellwarth-Iddings-Platzman (FHIP) theory.[18] More explicitly, Eq. (2) becomes[8]

$$\frac{m^*}{m_b} = 1 + \frac{\alpha}{6\sqrt{2\pi}} \mathrm{Im} \int_0^\infty dt \frac{t^2}{[D(t)]^{3/2}} [(1+\bar{n})e^{it}+\bar{n}e^{it}] , \tag{3}$$

with $\bar{n}$ the number of LO phonons,

$$D(t) = -i\frac{w^2}{2v^2}t\left(1+i\frac{t}{\beta}\right)+\frac{v^2-w^2}{2v^3}(1+e^{ivt}) , \tag{4}$$

where $\beta=T_D/T$ with $T_D=\hbar\omega_{\mathrm{LO}}/k_B$ (ω_{LO} is the LO-phonon frequency). In Eq. (4) v and w are the parameters describing the Feynman polaron model which are determined by a variational calculation[6] of the polaron free energy. It was pointed out in Ref. 8 that in the limit of zero temperature the expression (3) for m^*/m_b reduces to the Feynman polaron mass (e.g., for AgBr $m^*/m_b=1.33699$ for $\alpha=1.56$) and which is generally believed to provide a very good approximation to the actual (exact) polaron mass. Equation (2) results in a polaron mass that for sufficiently low temperature increases with temperature. For $\alpha \ll 1$ and $\beta \gg 1$ we can make a series expansion and find to lowest order in α and $1/\beta$

$$\frac{m^*}{m_b} = 1 + \frac{\alpha}{6}\left(1+\frac{9}{4}\frac{1}{\beta}+\cdots\right)+\cdots .$$

Note that this is the same result as was recently obtained by Fedyanin and Rodriguez[5] who obtained the polaron mass by calculating the change of the polaron free energy as function of the average polaron velocity.

The polaron mass as given by Eq. (2) is plotted in Fig. 1 (full curve) as a function of the temperature (which is scaled by $T_D = \hbar\omega_{\mathrm{LO}}/k_B = 201.4$ K) for AgBr. The experimental results for the polaron mass of Baxter, Ascarelli, and Rodriguez[12] from cyclotron resonance for the different samples are indicated by the various symbols (the same notation is used as in Ref. 12). In Fig. 1 we also show the mass corresponding to the Feynman polaron model [i.e., $(v/w)^2$] and the polaron mass as obtained from a relaxation-time approximation (RTA) to the polaron impedance function. The latter approximation is elaborated in detail in Ref. 8. The polaron mass derived from Eq. (3) (FHIP result) gives a better agreement with experiment than the polaron mass obtained from RTA and $(v/w)^2$. For the band mass of AgBr we have chosen the value (i.e., $m_b/m_e = 0.2110$ with m_e the bare electron mass) which was recently proposed in Ref. 17 on the basis of the magnetic field dependence[19] of the polaron cyclotron mass. The value of $m_b/m_e = 0.2148$, which was quoted in Ref. 20 and which is the generally accepted one, shifts the experimental results to lower polaron masses [note $m^*/m_b = (m^*/m_e)(m_e/m_b)$ and m^*/m_e is measured experimentally] and leads to less satisfactory agreement between theory (from FHIP) and experiment. Thus the new value $m_b/m_e = 0.2110$ for the band mass of electrons in AgBr is consistent with the experimental results on (i) the magnetic field[19] and (ii) the temperature dependence of the polaron cyclotron mass.

In conclusion, our calculation of the polaron mass based on Feynman's polaron model gives the right qualitative temperature behavior, in contrast with other polaron theories that predict a polaron mass that decreases with increasing temperature. Baxter, Ascarelli, and Rodriguez[12] explained the observed mass change in terms of a resonant interaction between conduction band and empty impurity states, where the interaction is mediated by acoustical phonons of energy 85 K. Hodby[15] pointed out that a more consistent explanation of the change in polaron mass with temperature can be given in terms of the nonparabolicity of the polaron band. The present analysis does not contradict Hodby's suggestion.

The agreement between the experimental and the FHIP-theoretical [Eq. (3)] polaron mass is rather qualitative than

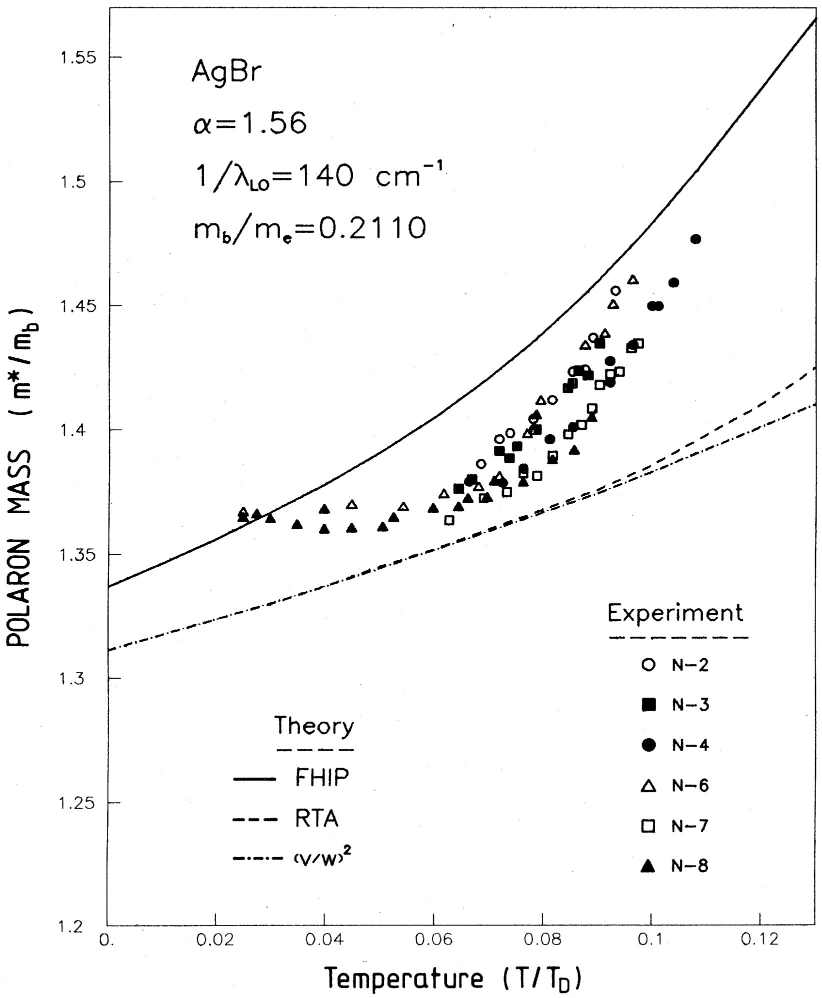

FIG. 1. Polaron mass vs the temperature for AgBr. The polaron mass is scaled by the band mass (m_b) and the temperature is scaled by the Debye temperature $T_D = \hbar\omega_{\mathrm{LO}}/k_B = 201.4$ K. Experimental results are from Baxter, Ascarelli, and Rodriguez (Ref. 12).

quantitative (see Fig. 1). The reason for the imperfect quantitative agreement may be that (1) other scattering mechanisms such as, e.g., acoustical phonon scattering, may play a role and (2) experimental accuracy problems in the determination of the position of the cyclotron resonance peak when the magnetic field is small may be important. In a recent study[19] of the magnetic field dependence of the polaron mass in AgBr and AgCl, it was found that the low magnetic field results could less accurately be determined experimentally than the high magnetic field results.

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