Comment on "Electron and hole polaron asymmetry in a two-band Peierls-Hubbard material"

K.Fesser, U.Sum, and H.Büttner
Physikalisches Institut, Universität Bayreuth, D-8580 Bayreuth, Federal Republic Germany
(Received 16 January 1991; revised manuscript received 20 February 1991)

The experimentally observed broken charge-conjugation symmetry in quasi-one-dimensional systems can be understood in an effective electron-phonon one-band Hamiltonian as a prototype model of these systems.

Recently experimental observations of intragap absorptions due to differently charged polarons in a quasi-one-dimensional substance have been reported.[1] The different charges lead to different locations of the localized levels of polarons within the gap, i.e., a broken charge-conjugation symmetry is found. For an explanation it has been shown in Ref. 1 that these features can be understood by a two-band Peierls-Hubbard model with $\frac{3}{4}$ filling and linear electron-phonon coupling; the fit to the data in Ref. 1, however, has been made only in terms of electron-phonon interactions.[2] We want to comment here that similar features also occur in simple one-band models with additional nonlinear electron-phonon without explicit electron-electron interactions. An example of such a model has been put forward by us[3] in connection with optical absorption experiments for one type of polarons only. A drastic shift of oscillator strength between various transitions has been found[4] in agreement with experiments. It is also predicted[5] that the mobility of various charged polarons scattered by acoustic phonons can be quite different.

Here we want to show that the asymmetry between electron and hole polaron as observed in Ref. 1 can also be interpreted within our approach. The starting point of our model is the Hamiltonian

$$H = H_{\mathrm{SSH}} + H_{\beta}$$

with H_{SSH} the Su-Schrieffer-Heeger Hamiltonian[6] and a new type of electron-phonon interaction H_{β}

$$H_{\beta} = \beta\alpha^2 \sum_{n,s} c^{+}_{n,s} c_{n,s} (u_{n+1} + u_{n-1} - 2u_n)^2,$$

which is treated perturbationally in the continuum limit. As described in detail in Ref. 3 the location of the intragap levels are given by

$$\varepsilon_{\pm} = \pm\omega_0(r) - \delta(r)$$

with the functions

$$\omega_0^2(r) = (1 - r^2)$$

and

$$\delta(r) = \tfrac{4}{3}\,\beta\Delta_0 r^2[\omega_0(r) - 2/5r^2]/(1 - r^2).$$

(Energies are measured in units of half the gap size $\Delta_0 = E_{\mathrm{gap}}/2$.) The parameter r is determined by minimization of the total energy, it describes the spatial width of the different polarons. This general result has several consequences that we want to discuss now.

First the symmetry of the polaron levels around the Fermi energy (midgap, which is set to zero numerically) is broken, and consequently the high-energy absorption line (B line in the notation of Ref. 1 corresponding to transitions of valence band to upper polaron level and lower polaron level to conduction band) is split; the amount of this splitting is equal to $2\,\delta(r)$. There is no splitting of the low-energy line (C line) due to occupancy and also none of the line corresponding to transitions between the intragap levels (A line).

The other consequence of the symmetry-breaking interaction is the fact that the value of the parameter r depends on the charge of the polaron under consideration. Since only a few numbers have been given in Ref. 4 we show in Fig. 1 the full dependence of r on the interaction parameter β. As one can see very clearly, the r values obtained for positively and negatively charged polarons are different, which in consequence yields different

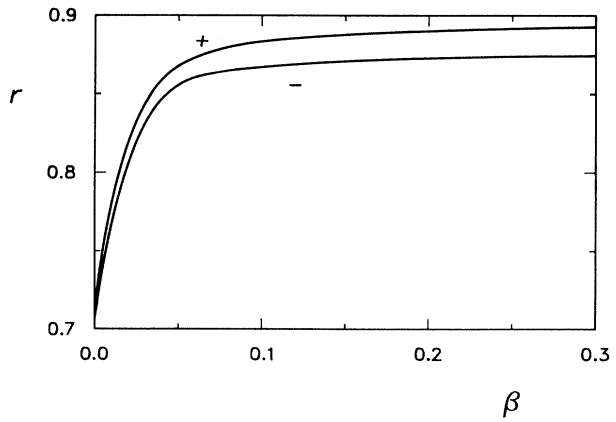

FIG. 1. The parameter r (see text) as function of the symmetry-breaking interaction strength β for positively (+) and negatively (−) charged polarons.

positions of the intragap levels according to the formulas discussed before and in agreement with the experimental findings in Ref. 1. The size of this effect is greater than the asymmetry splitting effect described before, numerically we find for a value of $\beta = 0.1$ a difference in r of 0.02, which in turn corresponds to a difference in the contribution of electron and hole polaron to the A line of 0.07, which is in excellent agreement with the experimental value 0.08 (in units of Δ_0) as given in Ref. 1.

In conclusion we want to stress that the experimental observations of broken charge-conjugation symmetry in quasi-one-dimensional systems as reflected in an enhanced oscillator strength and splitting of the B line as well as different absorption edges for positively and negatively charged polarons resulting in a splitting of all intragap lines can be incorporated in an effective one-band Hamiltonian with no explicit electron correlations as a prototype model of these systems. It would be of great interest whether the predictions for the mobility of Ref. 5 can be supported by further experiments.

This work was supported by the Deutsche Forschungsgemeinschaft, under SFB 213 (Topomak).

[1] J. T. Gammel, R. J. Donohoe, A. R. Bishop, and B. I. Swanson, Phys. Rev. B **42**, 10 566 (1990).
[2] J. T. Gammel and A. R. Bishop (private communication).
[3] U. Sum, K. Fesser, and H. Büttner, J. Phys. C **20**, L71 (1987); **20**, 2817 (1987).
[4] U. Sum, K. Fesser, and H. Büttner, Phys. Rev. B **38**, 6166 (1988).
[5] U. Sum, K. Fesser, and H. Büttner, Phys. Rev. B **40**, 10 509 (1989).
[6] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).