Localized versus band model of electrons in solids

Autor(en): **Fröhlich, H.**

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Localized Versus Band Model of Electrons in Solids

by **H. Fröhlich**

Department of Theoretical Physics, University of Liverpool

(29. IV. 68)

The sixtieth birthday of Georg Busch is a welcome opportunity for discussing certain electronic properties which in the current theoretical literature are frequently treated wrongly. I refer to the so-called 'small' polaron – an electron in a polar lattice in which its interaction with the lattice displacements is so large that its properties are very different from those of an electron in a substance in which the band model holds. Conditions for such possibilities were first mentioned by myself [1] in 1957; reference to some of the frequently occurring mistakes are found in Reference [2].

Under the circumstances in question, an electron is best described as localized around an ion with a certain chance of jumping to a neighbour. Such a state is described by a function φ_j which depends not only on the coordinates of the electron but also on those of the ions and it describes their displacement when the electron sits at a particular one, say near the lattice point $\boldsymbol{a}_j$ (cf. § 2 of Reference [2]). Crystal symmetry implies that a pure state is obtained from a linear superposition of localized states leading to a band state $\psi_{\boldsymbol{k}}$

$$\psi_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_j \varphi_j \, e^{i \boldsymbol{k} \boldsymbol{a}_j} ; \quad \varphi_j = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}} \, e^{-i \boldsymbol{k} \boldsymbol{a}_j} . \tag{1}$$

N is the number of sites. The $\psi_{\boldsymbol{k}}$ and φ_j form two orthogonal sets of functions.

In a many-body problem a wave function Φ of the whole system can be written as

$$\Phi = \sum_{\boldsymbol{k}} b_{\boldsymbol{k}} \, \psi_{\boldsymbol{k}} = \sum_j c_j \, \varphi_j \tag{2}$$

where the $b_{\boldsymbol{k}}$ and c_j are Fermi operators and

$$b_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_j c_j \, e^{-i \boldsymbol{k} \boldsymbol{a}_j} . \tag{3}$$

The expectation values

$$f(\boldsymbol{k}) = \langle b_{\boldsymbol{k}}^+ \, b_{\boldsymbol{k}} \rangle ; \quad g(\boldsymbol{a}_j) = \langle c_j^+ \, c_j \rangle \tag{4}$$

represent the distribution over wave vectors $\boldsymbol{k}$ (band model) or sites $\boldsymbol{a}_j$ (localized model) respectively. These distribution functions $f(\boldsymbol{k})$ or $g(\boldsymbol{a}_j)$ do not characterise the system sufficiently to work out the transport properties. Thus if the band model holds then clearly a correlation between the occupation of sites exists while different $\boldsymbol{k}$-occupations are not correlated in lowest order,

$$\langle b_{\boldsymbol{k}}^+ \, b_{\boldsymbol{q}} \rangle = 0 \quad \text{for} \quad \boldsymbol{k} \neq \boldsymbol{q} , \quad \text{band model.} \tag{5}$$

For the hopping model, based on localized states on the other hand, the correlation between occupation of sites is absent,

$$\langle c_j^+ \, c_l \rangle = 0 \quad \text{for} \quad \boldsymbol{j} \neq \boldsymbol{l} , \quad \text{localized model.} \tag{6}$$

But then using (3) and (6)

$$\langle b_{\boldsymbol{k}}^+ \, b_{\boldsymbol{q}} \rangle = \frac{1}{N} \sum_j \langle c_j^+ \, c_j \rangle \, e^{i (\boldsymbol{k} - \boldsymbol{q}) \boldsymbol{a}_j} \neq 0 , \tag{7}$$

except in thermal equilibrium, so that a $\boldsymbol{k}-\boldsymbol{q}$ correlation exists in contrast to the band model. Clearly when this latter holds then many of the standard transport formulae of the band model break down. Conditions for this breakdown are probably connected with the strength of interaction with the surrounding heat bath (thermal phonons, other electrons). When this breakdown has taken place then the normal band model formulae would lead to extremely small mean free path. These formulae are not valid, however, because they usually contradict relation (7), a feature which is frequently overlooked.

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