k-Space related properties in disordered solids

By K. Maschke, E. Mooser

Institut de Physique Appliquée, EPF-L, CH-1015 Lausanne

In honor of Martin Peter's 60th birthday.

Abstract. The eigenstates of a 1*d*-chain are calculated for a disorder potential $V(x)$, which is constructed from an array of Gaussian potentials with statistically varying amplitudes. The Gaussians are located on the points of a linear lattice with equal spacing. It is shown that in spite of a strong localization of the wave functions in real space, the mixing of the virtual-crystal Blochfunctions by disorder remains rather restricted in k-space. The dependence of the optical matrix elements on the localization of the wave functions in k- and r-space is discussed.

1. Introduction

The traditional description of electron states in crystals is determined by their translational symmetry. The eigenfunctions are Bloch states labeled by the quantum number k, which reflects the behavior of the states under a translation by a Bravais lattice vector. k is important for the description of physical processes. Thus, in the dipole approximation optical transitions, which will serve as example here, are governed by the k-selection rule, i.e. the transition matrix is diagonal in k.

Although the Bloch picture has been successfully used to solve many problems in solid state physics, several questions arise: In a real solid the translational symmetry is never perfect, not only because of its finite dimension, but also because of the presence in the bulk of structural and/or chemical disorder. While it is well known that the finite dimension of samples may give rise to surface states, the effect of disorder on the electron states is less clearly understood. In 1*d*- and 2*d*-disordered systems as well as for sufficiently strong disorder in 3*d*-systems it is generally accepted that the electron states are localized in real space [1]. In this case they are no longer described by their behavior under a spatial translation but by the decay of their amplitudes. Another description is therefore usually introduced, in which the quantum number k is suppressed [2] and optical transitions between two states can take place only when they overlap in real space. This description is unsatisfactory, since it cannot cope efficiently with the effects of different kinds and degrees of disorder.

1d-disorder is particularly critical in this respect, since the electron states are localized even in the presence of infinitesimally weak disorder. Optical transitions are then governed by the spatial overlap of the considered states ('r-selection rule') and not by the k-selection rule.

In the following we will consider 1d-disorder in some detail [3], to see whether the properties derived from the band structure of the ordered system are lost abruptly with the onset of disorder, or if its influence on electron states and optical transitions grows gradually with disorder.

2. Theoretical approach

We have calculated the eigenstates of a 1d-chain for a disorder potential $V(x)$, where

$$V(x) = \sum_n v_n(x - x_n) \qquad n = 1, 2, \ldots, N, \tag{1}$$

with

$$x_n = na.$$

The potentials v_n are Gaussian

$$v_n(x) = -a_n \sqrt{\alpha/\pi} \exp(-\alpha x^2), \tag{2}$$

and the amplitudes a_n vary statistically in the interval $(a_0 - W/2, a_0 + W/2)$.

Imposing periodic boundary conditions over the length Na we can write the eigenfunctions in terms of plane waves

$$\psi_i(x) = 1/\sqrt{Na} \sum_n c^i(K_n) \exp(iK_n x), \tag{3}$$

with

$$K_n = 2\pi \frac{n}{Na}. \tag{4}$$

In the ordered case ($W = 0$, virtual crystal) the eigenfunctions are Bloch functions $|lk\rangle$ which are specified by their k-vector and their band index l. To measure the influence of the disorder on the eignestates we develop the localized eigenfunctions ψ_n in terms of the Bloch functions $|lk\rangle$, i.e. we write

$$\psi_n = \sum_{lk} b_{lk}^n |lk\rangle. \tag{5}$$

According to equation (3) the optical matrix elements m_{nm} are

$$m_{nm} = \langle n| \vec{e} \cdot \vec{p} |m\rangle = \sum_l c^{n*}(K_l)c^m(K_l)K_l, \tag{6}$$

where $\vec{p}$ is the momentum operator and the polarization vector $\vec{e}$ is directed along

the chain. For comparison we have calculated the spatial overlap o_{nm} between the functions ψ_n and ψ_m

$$o_{nm} = \sum_i r_i^n r_i^m, \tag{7}$$

with

$$r_i^n = \sqrt{q_i^n} \tag{8}$$

and

$$q_i^n = \int_{(i-1/2)a}^{(i+1/2)a} |\psi_n(x)|^2 \, dx. \tag{9}$$

We have also determined the density of states $g(E)$ and the participation number $p(E)$. The density of states is given by

$$g(E) = \left\langle \sum_i \delta^\Delta(\varepsilon_i - E) \right\rangle, \tag{10}$$

where we have made use of the filter function

$$\delta^\Delta(E) = \begin{cases} 1 & \text{for } |E| \leq \Delta/2, \\ 0 & \text{else,} \end{cases} \tag{11}$$

which defines the energy resolution Δ. The brackets $\langle \cdots \rangle$ stand for configurational averaging. The participation number $p(E)$ measures the number of sites covered by the localized functions. It is given by

$$p(E) = \frac{1}{g(E)} \left\langle \sum_n \frac{1}{\sum_i (q_i^n)^2} \delta^\Delta(E - \varepsilon_n) \right\rangle. \tag{12}$$

3. Results

The results presented here have been obtained with the following parameter values: $a_0 = 23.75$ Ryd r_B, $W = 5.5$ Ryd, $a = 1r_B$, $\alpha = 6.25/r_B^2$, $N = 64$. The disorder was chosen strong enough, so that for a given sample size the localized wave functions do not change on going from periodic to antiperiodic boundary conditions. This is to assure that the results are fully representative of the description of an infinite disordered chain [4]. Results were obtained with a basis of 385 plane waves. The configurational average includes 50 samples. Other equivalent cases can be derived from the above parameter values by means of the scaling properties of the hamiltonian [3].

In Fig. 1 the first two bands of the unperturbed virtual crystal are shown. The density of states and the participation number in the presence of disorder are represented in Figs. 2 and 3, which show that the disorder mostly affects the
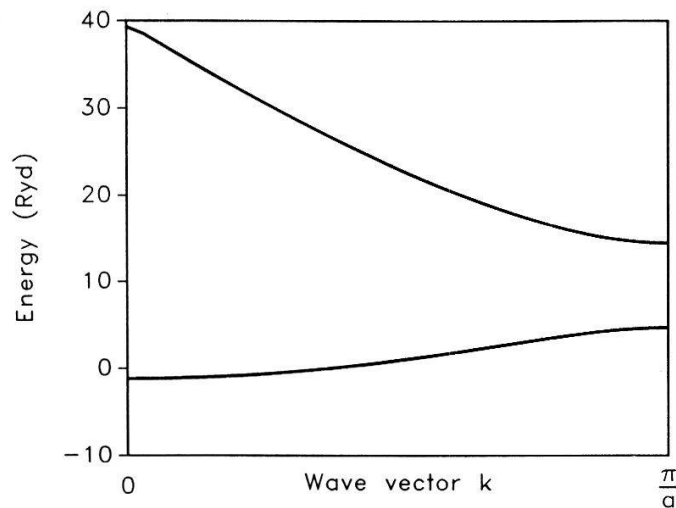
Figure 1
Band structure for the perfect virtual crystal ($W = 0$).

valence band states. The conduction band density of states still shows a large peak near the band edge similar to the $1/\sqrt{E}$-singularity of the perfect crystal. Away from the band edge the conduction band states rapidly become rather extended.

The different importance of the disorder for valence and conduction band states is most strikingly seen in Fig. 4, which shows the behavior of the averaged square of the expansion coefficients in equation (5). These coefficients are still rather well localized in k-space and peak along an $E(k)$-relation resembling the one of the virtual crystal, which thus turns out to be a good reference for the understanding of the disordered system. It should be noted that the k-vector refers to the extended zone scheme rather than to the first Brillouin zone. These results are in agreement with those obtained from the Anderson model [3].

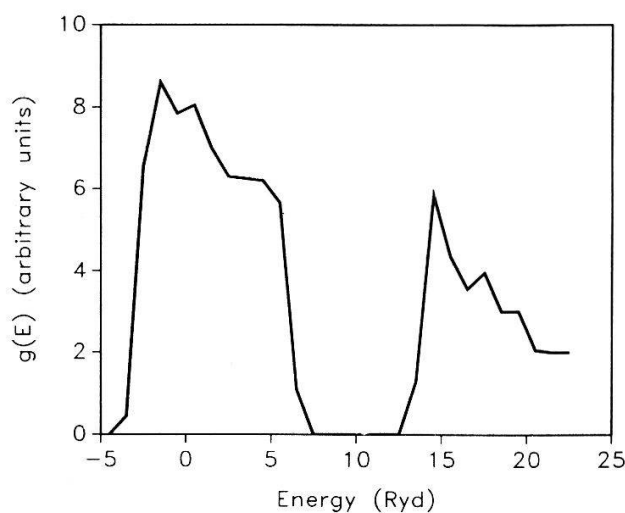Figure 4 implies that the k-selection rule is still important for optical

Figure 2
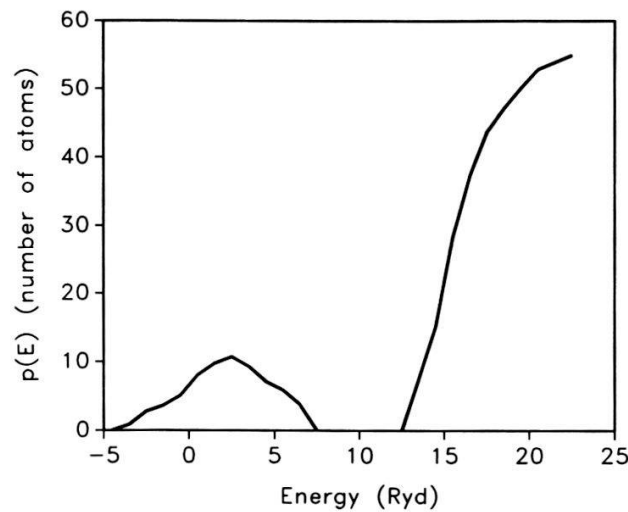Density of states for the disordered chain.

Figure 3
Participation number for the disordered chain.

transitions. This is confirmed by Fig. 5, in which the square of the optical matrix elements (full line) is shown as a function of the initial state energies for a fixed final state near the lower conduction band edge. For comparison we also show the corresponding spatial overlaps (dashed line). The difference between the two curves is quite striking. The behavior of the overlap matrix elements can be derived from the energy dependence of the localization (Fig. 3), which shows that the most localized states are found near the valence band edges. The peaking near the upper valence band edge of the transition probabilities calculated from the optical matrix elements (Fig. 5) is reminescent of the ideal virtual crystal, where it is described by a δ-peak.
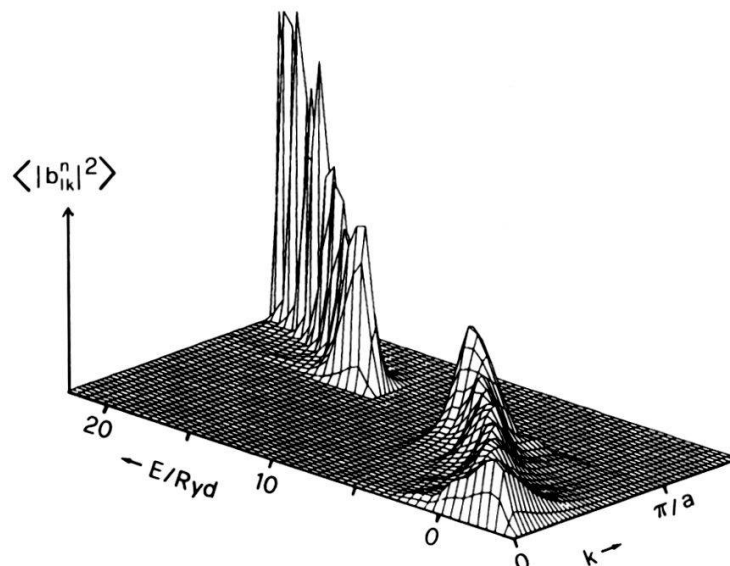

Figure 4
Decomposition of the localized states in terms of the eigenstates of the virtual crystal hamiltonian, see text. E is the energy of the localized states, k denotes the k-vector of the eigenfunctions of the virtual crystal.
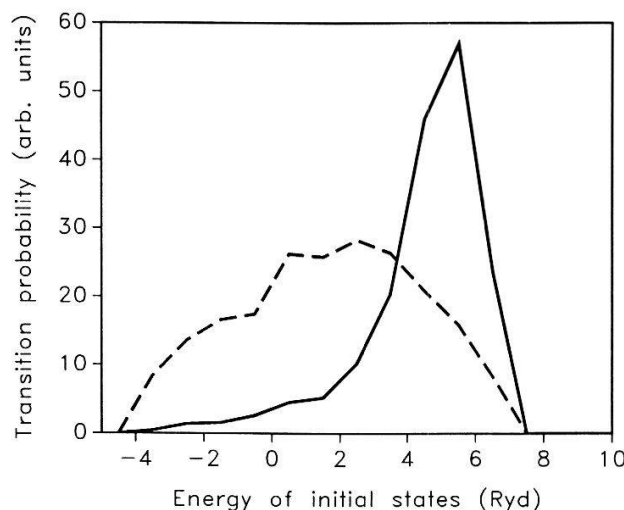
Figure 5
Dependence of the optical transition probability on the energy of the initial states. The final state energy $14\,\text{Ryd} < E_f < 15\,\text{Ryd}$ is chosen near the bottom of the conduction band. The full line is calculated from the optical matrix elements, the dashed line from the spatial overlap.

4. Conclusions

We have shown that even in the case of a 1d-disordered system, where the effects of disorder are expected to be largest, the k-space properties of the ordered virtual crystal are not destroyed abruptly. On the contrary, these properties disappear only gradually with increasing disorder. This is a consequence of the fact that the mixing of the virtual-crystal functions by disorder remains rather restricted in k-space, and only in the limit of very strong disorder will the localized states contain contributions from all Bloch functions with about equal weight. However, this limit is of little interest, since the wavefunctions are then localized on single sites.

As a consequence of the localization of the wavefunctions in k-space, the k-selection rule is still important for optical matrix elements, although the eigenfunctions may extend over a few sites only. Obviously with increasing disorder the k-selection rule is gradually replaced by the 'r-selection rule', which requires that states involved in a transition must overlap in real space.

Similar consequences can be expected for other properties like e.g. electronic transport, where the matrix elements of the momentum operator taken between the functions near the mobility edge are usually evaluated in the random phase approximation [5]. Our results imply that phase correlations within the wavefunctions in disordered systems still exist and ressemble those of the corresponding ordered system [6]. It would seem difficult therefore to justify the random phase approximation [7].

Acknowledgement

REFERENCES

[1] E. ABRAHAMS, P. N. ANDERSON, D. C. LICCIARDELLO, T. V. RAMAKRISHNAN, Phys. Rev. Lett. *42*, 673 (1979).
[2] J. TAUC, in: Optical Properties of Solids, ed. F. Abelès, North-Holland Publ. Comp., London, p. 277–p. 313, (1972).
[3] A more detailed discussion is found in: J. INGERS, K. MASCHKE, S. PRONNECKE, to be published in Phys. Rev. B.
[4] THOULESS, Phys. Rev. Lett. *39*, 1167.
[5] N. F. MOTT, Phil. Mag. *26*, 1015 (1972).
[6] I. MOULLET, K. MASCHKE, H. KUNZ, Journ. of Non-Crystalline Solids *77 & 78*, 17 (1985).
[7] K. MASCHKE, O. OVERHOF, to be published.