Duality between existence condition and construction procedure for interface states in a class of narrow-gap heterostructures

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Abstract

The problem for interface solutions in the quantum theory of heterostructures comprising narrow-gap semiconductors is reformulated in the language of commutative diagrams. By this way the theory of interface states in such heterostructures is naturally factorized in the two subproblems: (i) Criterion for the existence of interface states, and (ii) Their localization in the common energy gap; the solution of both of them being presented by the requirement for commutativity of the relevant diagrams. It is shown that these two problems are dual in the sense of categorical duality, the passing from the one commutative diagram to the other being realized by a (contravariant) functor $Op$.

1 Introduction

One of the characteristic features of mathematical physics is the use of abstract notions from mathematics in shedding light on physical problems and, along with this, the use of commutative diagrams by the discussion of general concepts in quantum physics [1,2]. However, the application of the latter technique to particular, even though important questions from the quantum theory of solids is rather inchoate. Thus, it is our aim in what follows to sift into the essence of such a particular problem making use of the language of commutative diagrams. More specifically, we shall speculate on the interrelation between the criterion for existence of interface states, on the one hand, and their localization in the common energy gap at the interface, on the other. To be definite, we shall consider an abrupt heterostructure comprising two different narrow-gap semiconductors in epitaxial contact.

In order to make the reading of the present paper as self-consistent as possible, let us sketch in the physical object under consideration. Heterostructures between narrow-gap semiconductors belong to the most important ingredients in solid-state electronics [3], and the two-band narrow-gap approximation, introduced initially by Keldysh [4] and Wolff [5], grew up lately in the method of choice by the discussion of their basic properties. Nowadays, there exists a variety of such approximations, and one could expect a new

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revival in this field due to recent experiments [6] providing strong confirmation of the wave-function hybridizations in narrow-gap heterostructures.

As a matter of fact, the theory of such heterostructures splits mainly in two quite different hybridization-based approaches: (i) considerations based on a Dirac-type equation (for a review see e.g. [7]), and (ii) a scattering-matrix theory [8,9] based on the hybridization procedure from the narrow-gap approximation of Pendry and Gurman [10,11] and subsequently generalized to account for the band-edge discontinuities in the energy-band profile at the interface [12,13]. It is this latter approach that we are here using as a starting point in what follows.

2 Preliminaries

To begin with, let us recall that a quantum theory of crystalline semiconductor may be characterized by the pair \( \{G, E_g\} \), \( G \) and \( E_g \) being the relevant crystal space group and the width of the energy gap, respectively. In what follows we are dealing with crystals with symmetry characterized by the presence of a mirror plane and a centre of symmetry in this plane. As regards the energy gaps, they are taken to be small and for simplicity, we suppose that they are opened in centre or edge of the corresponding Brillouin zone. (The generalization to gaps opened in a general position inside the Brillouin zone is straightforward [11]). By this way we consider heterostructures comprising two different crystalline materials of the above mentioned type, the interface being chosen parallel to the mirror planes characterizing the symmetry of the two crystals in epitaxial contact. For such heterostructures the \( S \)-matrix characterizing the interface as a scatterer

\[
S = \begin{pmatrix} r & \tau \\ t & \rho \end{pmatrix}
\]

takes the form [8]

\[
\begin{pmatrix}
\alpha \cdot e^{i\psi} & -i\sqrt{n(1-\alpha^2)}e^{i(\psi+\phi)/2} \\
-i\sqrt{1-n^2}e^{i(\psi+\phi)/2} & \alpha \cdot e^{i\varphi}
\end{pmatrix}
\]

where \( n \) is defined by the ratio of the group velocities of the flux-carrying Bloch waves on both sides of the interface; the real-valued positive quantities \( \alpha \) and \( \psi \) stand for the modulus and the argument of the reflection coefficient \( r \), respectively; and the real positive \( \varphi \) is the argument of the other reflection coefficient \( \rho \). The main result thus obtained in [8] is that in this case there may exists at most one interface state, the necessary and sufficient condition for its appearance being given by

\[
\tan \left( \frac{\psi + \phi_1}{2} \right) = \frac{1-\alpha}{1+\alpha} \cot \left( \frac{\varphi + \phi_2}{2} \right). \tag{2}
\]

Here \( \phi_j \ (j = 1, 2) \) are parameters characterizing the energy gap of the left \( (j = 1) \) and the right \( (j = 2) \) crystals.
3 Two rigorous results and their physical interpretation

The problem that faces us now is how to factorize the physical interpretation of (2) into two rigorously defined subproblems: (i) for existence of an interface solution and, if such a localized state does exist, (ii) for finding its position in the common energy gap. The reformulation of these problems in the language of commutative diagrams leads in a natural way to the nontrivial result that they are dual in the sense of categorical duality. However, the price of this is that in what follows we are forced to use a kind of mathematical manner, typical for the exposition of such results. Hence, both of the above subproblems have to be formulated as relevant propositions, followed by the rigorous proof of each of them.

As regards e.g. the first subproblem, its physical essence reduces to traversing the common energy gap in search for such values of energy, for which eq. (2) holds. Thus rigorously speaking, we arrive at our

**Proposition 1.** The criterion for existence of interface states is given by the requirement for the diagram

$$
\begin{array}{ccc}
E(\in E_g) & \xrightarrow{p_2} & \phi_2 \\
p_1 \downarrow & & \downarrow q_2 \\
\phi_1 & \xrightarrow{q_1} & I_1 = I_2 = I_0
\end{array}
$$

(3)

to be commutative, i.e.

$$q_1 \circ p_1 = q_2 \circ p_2$$

(4)

for some \(E \in E_g\), for which \(E = \text{dom}(q_1 \circ p_1) = \text{dom}(q_2 \circ p_2)\) is the energy of the interface state.

Let us only sketch the

**Proof:** To every value of the energy from the common gap \(E_g\) we juxtapose a corresponding value of \(\phi_j\) \((j = 1, 2)\) by the arrows

$$p_j : E \mapsto \phi_j \quad j = 1, 2.$$  

(5)

Then, defining the arrows \(q_j\) \((j = 1, 2)\) by

$$q_1 : \phi_1 \mapsto I_1 = \tan \left( \frac{\psi + \phi_1}{2} \right)$$  

(6)

$$q_2 : \phi_2 \mapsto I_2 = \frac{1 - \alpha}{1 + \alpha} \cot \left( \frac{\varphi + \phi_2}{2} \right),$$

we construct the composites of arrows \(q_1 \circ p_1\) and \(q_2 \circ p_2\). Traversing the common energy gap in search for such values of \(E \in E_g\), for which the diagram is commutative, we easily observe that this is just this \(E = E_{is}\) which is obtained as solution of (2). ■

The particular value of \(I_0(= I_1 = I_2)\) thus obtained is the starting point by the discussion of the second subproblem we are here interested in, namely, the localization of

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\(^2\)For the mathematical tools from the theory of commutative diagrams, needed for what follows, see e.g. [14].
the interface state in the common gap. Obviously, in order to answer this question it is sufficient that at least one of the compositions \( p_1^{-1} \circ q_1^{-1} \) or \( p_2^{-1} \circ q_2^{-1} \) do exist. As a matter of fact, for this particular case we shall prove a more general result in the next Proposition 2.

**Proposition 2.** To any commutative diagram (of the category of diagrams (3)) defining the existence of an interface state corresponds a dual to it (“opposite”) diagram which specifies the position of this interface state in the common energy gap.

**Proof:** The duality principle is a handy way to have (at once) the dual theorem and, in the categorical language, duality is defined by the process “Reverse all arrows” [14]. Thus, the diagram dual to our diagram (3) comprises the composite arrows \((q_j p_j)^{-1} = p_j^{-1} \circ q_j^{-1}\) \((j = 1, 2)\). On account of (5) immediately follow

\[
q_1^{-1} : I_0 \mapsto \phi_1 = 2 \cdot \tan^{-1} I_0 - \psi
\]

\[
q_2^{-1} : I_0 \mapsto \phi_2 = 2 \cdot \cot^{-1} \left( I_0 \frac{1 + \alpha}{1 - \alpha} \right) - \varphi.
\]

What remains to be done is to deduce the explicit form of the arrows \( p_j^{-1} \) \((j = 1, 2)\). From the hybridization procedure for two-band narrow-gap semiconductors [10,11] one obtains

\[
v_{j}^{in}(K_j - K_{0j}) - (E - E_{0j}) \frac{v_{j}^{in}}{v_{j}^{in}} + (V'_{j})_{+} \cdot e^{i\phi_j} = 0, \quad j = 1, 2,
\]

where \( K_j \) is the component of the Bloch-wave vector (for the relevant crystal) which is perpendicular to the interface; \( E_{0j} \) and \( K_{0j} \) designate the point in the Brillouin zone of the \( j \)-th crystal where the energy gap is opened; the quantity

\[
(V'_{j})_{+} = \langle a_j^+ \mid V'_{j} \mid a_j^- \rangle
\]

is the matrix element of this component \( V'_{j} \) of the relevant crystal potential which is responsible for opening the corresponding energy gap of the \( j \)-th crystal by the narrow-gap hybridization with the Bloch waves \( a_j^\pm \); and \( v_{j}^{in} \) are the group velocities of the incoming waves on both sides of the interface.

For the particular case of an energy gap opened in centre or edge of the Brillouin zone, \( K_j \) is complex-valued, its real part being \( Re(K_j) = K_{0j} \). Thus, we obtain from (8)

\[
p_j^{-1} : \phi_j \mapsto E = E_{0j} + v_{j}^{in}(V'_{j})_{+} \cdot \cos \phi_j, \quad j = 1, 2.
\]

From (7) ÷ (9) immediately follows that for the case under consideration both composite arrows \( p_j^{-1} \circ q_j^{-1} \) \((j = 1, 2)\) do exist and, consequently, the position of the interface state \( E_{is} \) in the common gap at the interface is defined in an unique way by

\[
E_{is} = \text{codom} I_0
\]

This completes the proof. ■

**Corollary 1.** Making use of e.g. the composite arrow \( p_1^{-1} \circ q_1^{-1} \) from (10) we obtain

\[
E_{is} = E_{01} + v_{1}^{in}(V'_{1})_{+} \cdot \cos(2 \tan^{-1} I_0 - \psi).
\]

**Corollary 2.** From the duality of the two problems - for existence of an interface state and for finding its position in the common energy gap - and as a result of their reformulation in terms of mutually opposite diagrams immediately follows that the passage from the one to the other is obtain under the action of a contravariant functor \( \text{Op} \).
4 Conclusions

We close with some remarks concerning the comparison between the present approach with the other one (based on a Dirac-type equation) we have referred to in the beginning.

Let us first of all mention that the name 'Dirac-type equation' is somewhat misleading for this is only a suggestion that it is formally obtained from the relativistic wave equation of Dirac by replacing the universal constant 'velocity of light $c$' by the so called 'interband velocity matrix element $v$' [15]. Hence, the relevant theory of such interface states has nothing to do with the relativistic-quantum theory of interface states ([16], see also [17,18]).

In addition, it is worth noting that the present alternative approach seems to be more convenient by the discussion of the essence of basic problems in the two-band narrow-gap quantum theory of semiconductor heterostructures.

An instructive example in this direction is the duality between existence condition and construction procedure for the particular above discussed problem. It may be also considered as a nice example for unusual but useful application of a modern mathematical tool— the notion of of commutative diagrams to a particular problem from the theory of solids. It is worth nothing that, as regards the scattering-theoretical approach to heterojunction problems, it is important to take into account the specific features characterizing the scattering by potentials with different finite asymptotics for $x \to -\infty$ and $x \to +\infty$, respectively [19, 20]. What is more, as regards the use of heterojunction $S$- matrices (like those from [8]) as a starting point, the situation is even additionally complicated due to the need to take into account Bloch waves in the two different crystals in epitaxial contact and the relevant generalizations of the properties characterizing a heterojunction $S$- matrix.

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