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ELECTRONIC ENERGY LEVELS OF MULTILAYER STRUCTURES WITH THE RENORMALIZATION METHOD.

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Abstract. We summarize here the relevant features of the renormalization method for the study of the electronic energies of multilayer structures. With a suitable use of the translational symmetry in planes parallel to the growth axis, the method becomes a very simple and effective tool . As an exemplification, results for the InAs-GaSb superlattice are presented.

1. Introduction

The renormalization method with a mixed real-space reciprocal-space representation, is appearing as one of the most powerful procedures for the study of multilayer structures such as surfaces, heterostructures, quantum wells, multiple quantum wells and superlattices.

Only in the last decade this method has been developed for the evaluation of the electronic states of ordered as well disordered crystals, and several equivalent formal expressions have been proposed for it [1,2]. Very recently it has been emphasized the analogy between the renormalization method and the recursion method [3,4] : the analogy goes well beyond the common algebraic deduction at the basis of the two methods, and it is ultimately linked to the concept of the effective reduced hamiltonians which are built for them, from the same projective procedure.

We disregard here the technical details of the renormalization method, which have been well presented elsewere [3-5] ; we pick up only some important concepts and

underly the strong opportunity that this method gives, to treat in a unifying way, any kind of layer structure. Finally, as an exemplification, we present some results for the InAs-GaSb superlattice.

2. The method

The renormalization method consists in a systematic reduction of the degrees of freedom of a given system, which allows to mimic the original system with a smaller one with renormalized interactions. This is of practical use only if the reduced hamiltonian has the same form as the original one so that the procedure can be iterated without encountering the difficulty connected with " induced interactions ". This difficulty is easily overcome for multilayer structures by exploiting their two dimensional symmetry in the planes parallel to the interfaces; we thus reduce the three dimensional system to a linear chain on which the renormalization approach can be carried out exactly. Let us clarify this point with reference to the (001) atomic planes of the zincblende type semiconductors: these planes are alternatively composed by anions and cations. From the n independent orbitals ϕ_i (i=1,...,n), in each plane, let us construct the following two dimensional "layer" Bloch sums $\{ \Phi_{l,i}(\mathbf{r},\mathbf{q}) \}$

$$\Phi_{l,i} = \frac{1}{\sqrt{N_2}} \sum_{\tau_n} e^{i\mathbf{q}\cdot\tau_n} \phi_i(\mathbf{r} - \tau_n) \qquad (1)$$

where the sum runs over the N_2 translation vectors τ_n of the layer l and $\mathbf{q}$ is the two dimensional Bloch vector with components k_x and k_y. On this basis , for any $\mathbf{q}$, the Hamiltonian is represented by a block tridiagonal matrix wich formally desribes a linear chain with n orbitals per site: we are thus faced with a unidimensional system. We have for example a one sided semiinfinite linear chain for a surface, two semiinfinite chains with an internal finite chain for a single quantum well, and we have at least two finite chains with periodic boundary conditions for a superlattice.

The microscopic description of the composing crystals is done in terms of localized orbitals with any arbitrary range of interaction. If the interactions are confined to nearest neighbor atoms, the renormalization eliminates alternate atomic layers; if the interactions are extended up to m atomic layers, the renormalization eliminates alternate

"principal layers" each composed by m atomic layers. In the case of an ideal surface, we have for any **q**, the following starting hamiltonian

$$H_{\mathbf{q}} = \sum_{\substack{n=1,\infty \\ \alpha,\beta}} \{A_{\alpha\beta} |\Phi_{n,\alpha}\rangle\langle\Phi_{n,\beta}| + B_{\alpha\beta} |\Phi_{n,\alpha}\rangle\langle\Phi_{n+1,\beta}| + C_{\alpha\beta} |\Phi_{n+1,\alpha}\rangle\langle\Phi_{n,\beta}|\} \tag{2}$$

where the greek symbols indicate the orbitals of a given layer n. In the case of a superlattice with N atomic layers in the unit cell, for any $(\mathbf{q},k_z)$ the starting hamiltonian takes the form

$$\begin{aligned} H_{\mathbf{q},k_z} = & \sum_{n=1}^{N} \sum_{\alpha,\beta} \{A_{n,\alpha\beta} |\Phi_{n,\alpha}\rangle\langle\Phi_{n,\beta}| + \sum_{n=1}^{N-1} \sum_{\alpha,\beta} B_{n,\alpha;n+1,\beta} |\Phi_{n,\alpha}\rangle\langle\Phi_{n+1,\beta}| \\ & + \sum_{n=1}^{N-1} \sum_{\alpha,\beta} C_{n+1,\alpha;n,\beta} |\Phi_{n+1,\alpha}\rangle\langle\Phi_{n,\beta}| + \\ & + \sum_{\alpha,\beta} B_{1,\alpha;N,\beta} |\Phi_{1,\alpha}\rangle\langle\Phi_{N,\beta}| + \sum_{\alpha,\beta} C_{N,\alpha;1,\beta} |\Phi_{N,\alpha}\rangle\langle\Phi_{1,\beta}| \} \end{aligned} \tag{3}$$

where the corner matrices B_{1N} and C_{N1} contain the exponential term $\exp(ik_z d)$ required by the boundary conditions.

We can now iteratively renormalize the above hamiltonians defining at each step the following effective new hamiltonian $H^{(R)}$:

$$H_s^{(R)} = H_s + H_{int} \frac{1}{E - H_{s'}} H_{int}^{+} \tag{4}$$

where H_s is the hamiltonian to be renormalized, defined in the space S; H_{int} is the interaction term which connects the space S whith the space S' (described by the hamiltonian $H_{s'}$) to be eliminated.

In the case of a semiinfinite system the iterations are continued up to the reachment of the fixed point: in the flat band approximation, if this is achieved in N steps, the surface layer interacts with the layer 2^N far away (in the units of interlayer separation),

and this assures that the procedure converges rapidly. In the case of a superlattice with $N=N_A+N_B$ layers, the internal degrees of freedom are decimated with the small number of iterations $\log N_A + \log N_B$.

3. The InAs-Gasb superlattice.

As an example we consider here the electronic strucure of the InAs-GaSb (001) grown superlattice. In this system the large valence band offset allows to taylor the optical gap over a wide range, just by varying the superlattice period. This is shown in Fig.1 which displays the band structure evolution as the number of atomic planes in the unit cell increases.Shaded regions are the projection of the superlattice band dispersion along the direction of the growth axis (the other components of the Bloch wave vector are zero). For short period superlattices, in the energy region between the top of the valence bands of InAs, and the bottom of the conduction bands of GaSb, the superlattice bands can be either electron like states confined in InAs, or hole like states confined in GaSb. As the cell dimension increases, the hole like subbands raise toward the top of the GaSb valence band (at 0.57 eV), and the electron like subbands approach from above the bottom of the InAs conduction band (at 0.41 eV); these energy levels are indicated by dashed lines in Fig.1. For $N_A=N_B \geq 64$ the electron like and hole like states mix, and the superlattice becomes semimetallic. This transition has been analized in detail in ref.[6].

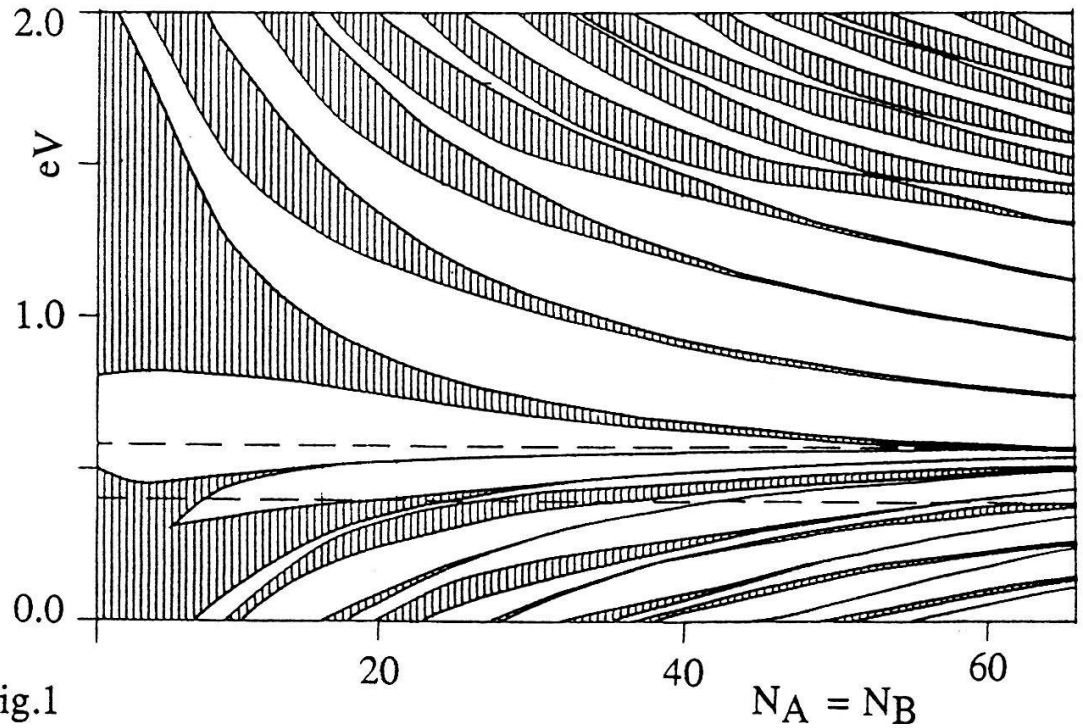
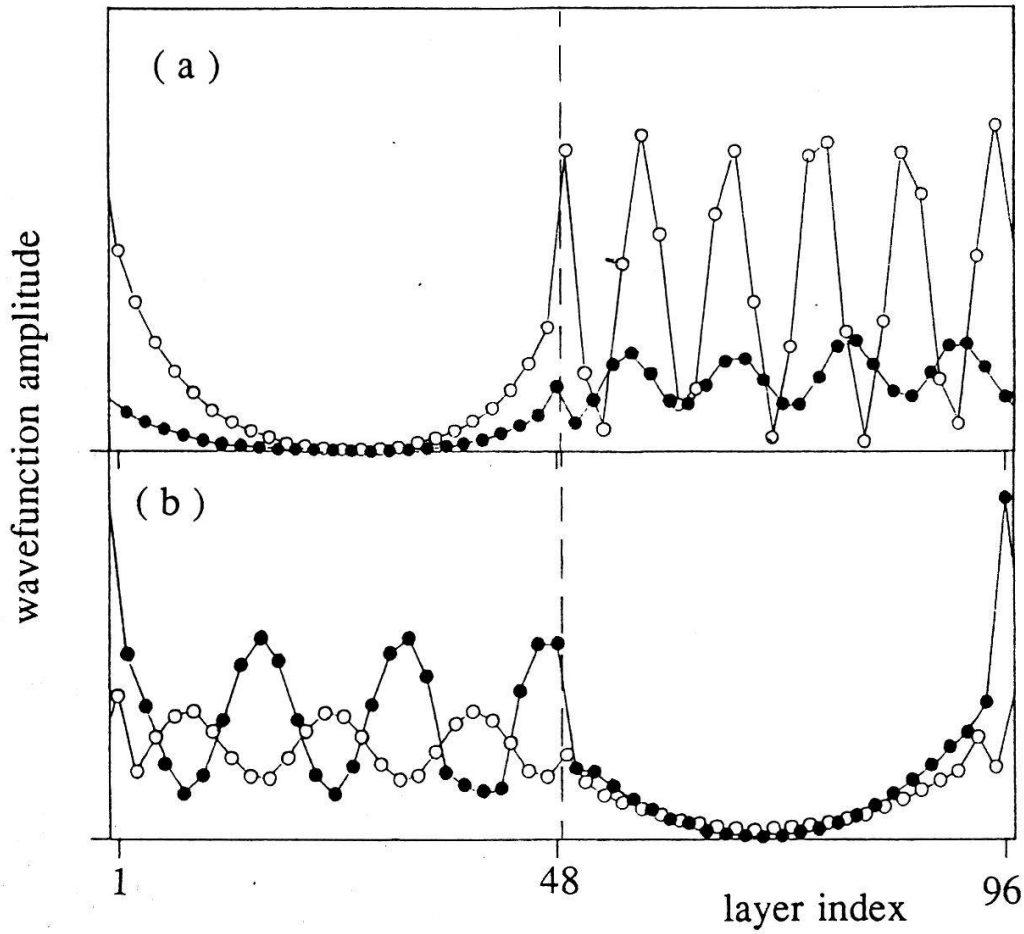


Fig.1

Fig.2 displays the localization properties of the E4 state (fourth electron like state from below) and the HH6 one (sixth heavy hole like state, from above), for $N_A=N_B$ = 48.Full and empty dots indicate the wavefunction amplitudes on cations and anions respectively; layers from 1 to 48 are InAs, and from 49 to 96 are GaSb. The state HH6 (Fig.2.a) presents the 5-nodes structure typical of the 6th state in a quantum well; it has strong p-orbital character and is mainly localized on GaSb. In the E4 state (Fig.2.b), the 3-nodes structure is less pronounced; however it has prevailing s-orbital character and shows confinement on InAs.

Fig.2



4. Conclusions

Due to its formal and technical simplicity, the renormalization method seems indeed a very powerful tool for the evaluation of the electronic structure of multilayer structures. Among the pleasant features of the method we stress that it exploits a fully microscopic description of the composing crystals, that no limitation exists in the size of the superlattice unit cell and the possibility of overcoming the flat band approximation toward self-consistent calculations.

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