Photon Absorption in Periodically Regimented Nanostructures

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“The achievement of a well-defined superlattice structure with a period of, say, 100 Å will require considerable effort even with the use of the most advanced epitaxial thin-film technologies.”

“Although it may be a formidable task to construct the proposed superlattice, we believe that efforts directed to this end will open new areas of investigation in the field of semiconductor physics.”

A comment by L. Esaki in 1987:

"The original version of the paper was rejected for publication by Physical Review on the referee's unimaginative assertion that it was 'too speculative' and involved 'no new physics'.”
Applications of 1-D Superlattices
(Daily lab work in 2012)

- Quantum cascade lasers
- Quantum cascade LEDs
- VLWIR (very long wavelength infrared detectors)
- Thermoelectric applications
- ...

Could we obtain novel applications from 2-D or 3-D superlattices?
Experimental Work to Obtain 2-D and 3-D Superlattices


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How to study these systems?


\[
\left[ -\frac{\hbar^2}{2m^*(r)} \nabla^2 + V(r) \right] \varphi(r) = E \varphi(r)
\]

\[
V(r) = V_x(x) + V_y(y) + V_z(z)
\]

Advantages:
- Simple picture to understand the system.
- The solutions are analytical, and they could be related to the 1-D Kronig-Penney model.

Drawbacks:
- The interaction in diagonal directions is greater than in the real system (nearest neighbour approach).
- The space-dependent effective mass kinetic energy operator is not separable. Some approximations within this approach are not right.
How to study these systems?


From a qualitative point of view there are very good issues commented on in these first works:
- Miniband structure (degeneration, wave functions structures...)
- Density of states

Nevertheless, because of the non-separability of the kinetic energy operator, there are some issues that should be clarified:
- Crossings between minibands, caused by the independence of the 1-D solutions

Therefore, another approach should be used.
Normalized Plane-Wave Approach

\[ \psi(x, y, z) = \frac{1}{\sqrt{L_x L_y L_z n_x n_y n_z}} \sum a_{n_x, n_y, n_z} e^{i(k_{n_x}x + k_{n_y}y + k_{n_z}z)} \]

Advantages:
- The real potential could be used, as well as the one used by O. L. Lazarenkova and A. Balandin
- The space-dependent effective mass in kinetic energy operator can be used
- There is no problem with matching conditions between dots and barriers, even with different effective masses
- The solutions should be physically reasonable

Drawbacks:
- It is not analytical
- The results are obtained with a certain error because the expansion should be cut at a certain term (like the cut-off energy in the talk given by Professor Matt Probert)
Normalized Plane-Wave Approach

The Schrödinger Equation:

\[
- \frac{\hbar^2}{2} \left[ \nabla \frac{1}{m(\vec{r})} \nabla \right] \Psi_{\vec{q},n}(\vec{r}) + V_{\text{strained}}(\vec{r}) \Psi_{\vec{q},n}(\vec{r}) = E_n(\vec{q}) \Psi_{\vec{q},n}(\vec{r})
\]

Features:
- This is a periodic Hamiltonian. The Floquet-Bloch theorem gives the structure of the wavefunctions:

\[
\Psi_{\vec{q},n}(\vec{r}) = \eta_{\vec{q},n}(\vec{r}) e^{i\vec{q} \cdot \vec{r}}
\]

This defines a Q-space, a space where each point is an eigenstate of the hamiltonian, in the same manner than the K-space for regular crystals.

Once \( \vec{q} \) is chosen, the Schrödinger equation is solved. The set of eigenenergies is represented. Changing \( \vec{q} \) a new set of eigenenergies is obtained. The representation of these results gives the miniband structure.
The Q Space

The dimensionality of the space depends on the periodicity of the system.

A n-D superlattice has a n-D Q space

FIG. 3. (Color online) Mini-band structure of the system having a 4 nm side length in a supercell of 8 nm side length. Solid lines are obtained by means of the plane wave method. Dotted lines are the solution of the three-dimensional Kronig-Penney model as reported by previous authors.

FIG. 4. (Color online) 3D representation of a supercell with an 8 nm side length in the Brillouin zone of a (001) oriented supercell. Green solid lines depict the energy bands of an 8 nm supercell, and red dashed lines are for the 4 nm supercell. Dotted lines illustrate the solution of the Kronig-Penney model as reported by previous authors.

FIG. 5. (Color online) Mini-band structure of the system having an 8 nm side length in a supercell of 10 nm side length. Solid lines are obtained by means of the plane wave method. Dotted lines are the solution of the three-dimensional Kronig-Penney model as reported by previous authors.
Photon Absorption

The features of the wavefunctions and eigenstates influence the selection rules for optical transitions between the minibands. These rates are obtained using the following formula:

\[
\alpha_{n_i \rightarrow n_f}(\hbar \omega_{op}) = \frac{\pi |e|^2}{n_e c \epsilon_0 m_0^2 \omega_{op}} \int Q_{\text{space}} f(E_{n_i})\left[1 - f(E_{n_f})\right]
\]

\[
\times \left| \xi \cdot \sum_l \hbar \tilde{k}_l c_l^* (q_l, n_f) c_l (q_l, n_i) \right|^2
\]

\[
\times \delta(E_{n_f} - E_{n_i} - \hbar \omega_{op}) p_q dq
\]

There is a dependence on light polarization. The selection rules only allow transitions keeping the wave vector constant.
- The normalized plane-wave method gives wavefunctions as a sum of waves with several wave vectors.
- Just the coefficients for each wave vector should be multiplied between them. There is no mixing between components.
Results

These systems often provide results with a stepped threshold in photon absorption.

This is not exclusive of cubic/cuboid quantum dots neither exclusive of 3-D regimented systems. It could be useful to develop photodetectors like QDIPs.

Advantages:
- Prediction of interesting behaviour of these systems.
- It could be a guide for experimentalist to ascertain if these systems might be useful or not.

Drawbacks:
- The technology for manufacturing these systems is not well developed nowadays.
- It might happen that you could have referees’ unimaginative assertions that it is “too speculative” and involve “no new physics” 😊
Nevertheless... we might be on the right way

Recent papers confirm the goodness of these approaches to study these systems. Some comparisons with experimental results have been carried out.

Nanopores leave quantum dots between pores. It is possible to manufacture these systems. It is possible to theoretically study these systems, and it is also possible to compare with experimental results.

Nice agreements are found.

Conclusions

- We have presented the theory of photon absorption in periodically regimented nanostructures.

- We have shown that some simplifying approaches are not suitable to investigate in depth these systems.

- We have shown the advantages of using the normalized plane-wave method.

- We have shown some obtained miniband structures and photon absorption profiles.

- We have shown some results obtained by other groups supporting this framework to obtain, at least, qualitative behaviours of the systems.

Thanks for your attention/patience! 😊