File name: Electron wavefunction, derived formula

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Formulas are derived based on PRB, 46, 6969(1992) & JAP, 72, 4714(1992)

**Updated: Momentum matrix P is calculated by Eg and m\*, not by Ep**

# The k·p theory for 2 band model

In Bloch Theorem, wave function is given by 

Apply to Schrodinger equation:  (1)

If only two strongly interacting non-degenerate bands are considered (e.g**., conduction band and light hole valence band**), we call them class A as in Lowdin’s method.

Assuming, where ac, av are so-called envelope function. substitute into equation (1), we have



A general solution is



And total wavefunction will be , which is the superposition of each component

 (1-1)

 (1-2)

k has positive imaginary part for electron wave in energy gap and negative part for hole wave in energy gap

 , could be phenomenally determined by  (1-3)

Picture2.tifPicture3.tif

## Basic expression

From left to right, the wavefunction is (1-4)

## Continuity at interface

 (1-5)

 (1-6a,b)

For next layer ,  (1-7a)

For previous layer,  (1-7b)

Both approaches should be equivalent, but (1-7a) is more intuitive and more convenient for coding.

The matlab command “inv” or”\”can do inverse calculation at the cost of less accuracy. The formula is:

 (1-8a,b)

## Calculate each (A, B) pair at interface

 (1-9)

The expression for the last layer should be paid care due to the absence of d.  (1-10)

 (1-11)

## Boundary condition



For MQW, there should be no incoming waves from both sides, M22=0

For SL, the wavefunction should be periodic with only phase difference. trace(M)/2<=1;

For electron wave,  (1-12a)

for hole wave,  (1-12b)

## Normalization

 (1-13)

## GaSb/InAs/GaSb

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| material | Ec | Eg | m\*/m0 | P(cm/s) | source |
| GaSb | 0.83 | 0.68 | ml 0.05 | 1.066e8 | PRB,46, 6969 |
| InAs | 0 | 0.36 | mc 0.027 | 1.068e8 | PRB,46, 6969 |

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# 1 band model for heavy hole valence band

For a Schrodinger equation of the form:

A general solution will be 

Wave vector is given by:



Boundary conditions:  ,are continuous at the boundary

 (1-14)

## GaSb QW

### Ground and 1st excited state

 