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TRSS: a new version of program TRS for a different geometry

Joachim Schmitz [1], Hans-Rainer Trebin [2]
Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, W-7000 Stuttgart 80, Germany

and

Ulrich Rössler [3]
Institut für Theoretische Physik, Universität Regensburg, Universitätsstrasse 31, W-8400 Regensburg, Germany

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Quantum resonances in the bands of semiconductors under uniaxial stress provide very detailed information on the band parameters. However, the analysis of experimental data is difficult. Computer programs based on an adequate theoretical model make this task easier. Program TRSS calculates energy eigenvalues, wave functions and oscillator strengths for direct inter- and intraband dipole transitions. The magnetic field is applied parallel to the [001] crystal axis while the uniaxial stress is directed perpendicular [100] to it.

NEW VERSION SUMMARY

Title of new version: TRSS

Catalogue number: ACGS

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Reference to original program: Comput. Phys. Commun. 66 (1991) 308; *catalogue number*: ACBH

Authors of original program: J. Schmitz, H.-R. Trebin and U. Rössler

Does the new version supersede the original program? no

Licensing provisions: none

Computer: VAX II/GPX; *Installation*: Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, W-7000 Stuttgart 80, Germany

Operating system under which the new version has been tested: VAX/VMS 4.6

Programming language used in the new version: standard FORTRAN 77

Memory required to execute with typical data: 434 Kbytes

No. of bits in a word: 32

Peripherals used: terminal, disk

No. of lines in distributed program, including test data, etc.: 5207

Separate documentation available: TRS User's and Programmer's Guide: *no. of pages*: 76: *available from*: CPC Program Library, or Joachim Schmitz, Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, W-7000 Stuttgart 80, Germany, joa@ds0ita51.bitnet

Keywords: narrow-gap semiconductors, zincblende lattice, Landau levels, uniaxially stress parallel to magnetic field, effective Hamiltonian, invariant expansion, eightfold space of valence band and lowest conduction band, normal and inverted bands, energy eigenvalues, eigenvectors, direct inter- and intraband dipole transitions, oscillator strengths, Γ-point, [001] and [100] crystal axis, uniaxial stress perpendicular to magnetic field

[1] joa@ds0ita51.bitnet
[2] trebin@ds0ita51.bitnet
[3] roessler@vax1.rz.uni-regensburg.dbp.de

Nature of physical problem
An effective Hamiltonian constructed by invariant expansion is used to calculate Landau levels and wave functions in narrow-gap semiconductors with a zincblende or diamond lattice under uniaxial stress [4]. It is based on an eightfold space of uppermost valence and lowest conduction bands at the center of the Brillouin zone and its vicinity. The wave functions are further used to calculate the oscillator strengths of direct inter- and intraband dipole transitions. Thus the TRSS program is a valuable tool for the experimentalist to analyze quantum resonances measured in semiconductors.

Method of solution
The matrix elements of the Hamiltonian are set up one by one according to the equations derived from the theory [2,3]. Then the resulting matrix is diagonalized using Householder's reduction followed by the QL method. Energy eigenvalues and eigenvectors are further used in calculation of oscillator strengths.

Reasons for the new version
Adaptation for a different geometry

Restrictions on the complexity of the problem
The dimensions of arrays are set to include Landau levels with oscillator quantum number up to $n_a \leq 39$. Adaptations are easily made. Due to the limitations in the Kane-modell [1] and the underlying perturbation theory the program is only suitable for eigenstates in the vicinity of the Γ-point. Transitions are restricted to direct dipole transitions. All calculations are based on a geometry with magnetic field parallel to the [001] crystal axis and uniaxial stress applied parallel to the [100] crystal axis.

Typical running time
Same as for program TRS

Unusual features of the program
TRSS contains a subroutine which clears the screen of the terminal before displaying a new page of text. This action is not essential to the operation of the program and may be entirely omitted. In order to preserve the intended screen display it must be adapted to the specific device used.

References

[1] E.O. Kane, in: Semiconductors and Semimetalls, vol. 1, eds. R.K. Willardson and A.C. Beer (Academic, New York, 1966) p. 75.
[2] H.-R. Trebin, U. Rössler and R. Ranvaud, Phys. Rev. B 20 (1979) 686.
[3] H.-R. Trebin, W. Wolfstädter, H. Pascher and H. Häfele, Phys. Rev. B 37 (1988) 10249.
[4] G.L. Bir and G.E. Pikus, Symmetry and Strain-Induced Effects in Semiconductors (Wiley, New York, 1974).

LONG WRITE-UP

Detailed information on the band parameters of a semiconductor can be obtained from quantum resonances in uniaxially stressed crystals. To this end the experimental data must be analyzed on the basis of a theoretical model. This model was provided by Trebin and Rössler [1,2] for narrow-gap semiconductors with a zincblende lattice. It is based on an effective Hamiltonian constructed by invariant expansion. A concise description of the theory has already been given in ref. [3].

The secular problem posed by this Hamiltonian may be solved for any geometry, i.e. with no regard for the directions of magnetic field and uniaxial stress relative to the crystal axes. However, in experiments only a few selected configurations are used corresponding to high-symmetry directions. Incorporating any of these into the equations greatly simplifies the Hamiltonian and the secular problem. Trebin et al. [1] set up the Hamiltonians for magnetic fields *parallel* to uniaxial stress applied along the [001], [111], and [110] crystal axes. Program TRS [3] is based upon the geometry where both magnetic field and stress are directed parallel to [001].

Later, Trebin et al. [2] showed that under crossed magnetic field and stress the Landau levels of semiconductors are separated much stronger with stress yielding more insight into the band structure than in the parallel configuration. They compared geometries where the magnetic field is directed along the [001] crystal axis and uniaxial stress either parallel or *perpendicular* [100] to it. Surprisingly, the modifications to the Hamiltonian – though essential – are minor. Moreover, the selection rules for direct inter- and intraband transitions stay the same. Therefore it was possible to adapt program TRS to this new configuration without major changes. The new program is given the name TRSS. Essential adaptations are made in subroutine MATRIX where the matrix Hamiltonian is built up. All other adaptations concern text strings of the interactive menu displays and descriptive comments in the FORTRAN code.

Since no further changes are necessary, all input and output data formats remain the same. The separate documentation "TRS User's and Programmer's Guide" is valid throughout for program TRSS as well. The only differences are visible in the interactive menu displays and naturally in the results of the calculations. Two pages from the test run are shown in this paper, the test run input being identical for both TRS and TRSS.

References

[1] H.-R. Trebin, U. Rössler and R. Ranvaud, Phys. Rev. B 20 (1979) 686.

[2] H.-R. Trebin, W. Wolfstädter, H. Pascher and H. Häfele, Phys. Rev. B 37 (1988) 10249.

[3] J. Schmitz, H.-R. Trebin, and U. Rössler, Comput. Phys. Commun. 66 (1991) 308.

TEST RUN OUTPUT

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*** LANDAU-LEVELS IN ZINCBLENDE-TYPE SEMICONDUCTORS ***

INSB.DAT


REPRESENTATION  2  -  eigenvalues and eigenvectors from 28V 14C 14S functions


Eigenvalues

        437.4044       426.4820       419.6620       408.0960       401.0707       388.3464       380.9472       366.8944

Eigenvectors    1             2              3              4              5              6              7              8

     28C  0.8268   25C -0.8212    24C  0.8195    21C -0.8354    20C  0.8351    17C  0.8490    16C  0.8498    13C -0.8623
     60V  0.4441   45V  0.4208    52V  0.4247    37V  0.4095    44V  0.4149    29V -0.3923    36V  0.3992    21V  0.3666
     50V -0.2484   55V -0.2560    42V -0.2368    47V -0.2497    34V -0.2289    39V  0.2406    31V  0.2232    26V -0.2362
     55V  0.1827   50V -0.1843    47V  0.1911    42V -0.1994    39V  0.2062    34V  0.2166    26V -0.2170    31V -0.2281

Eigenvalues

        358.9059       343.2072       334.3751       316.4432       306.4028       285.0692        -0.5987        -1.6677

Eigenvectors    9            10             11             12             13             14             15             16

     12C  0.8644    9C  0.8774     8C  0.8811     5C  0.8975     4C  0.9036     1C  0.9294     4V  0.9219     5V -0.7137
     28V  0.3747   13V -0.3268    20V  0.3362    10V  0.2918     7V  0.3049     2V  0.3397    12V -0.2757    10V -0.5420
     23V  0.2434   18V  0.2600    15V  0.2691     5V -0.2576    12V  0.2673     7V  0.1216     7V  0.1943    12V  0.2152
     18V -0.1989   23V  0.2102    10V -0.1695    15V  0.1816     2V -0.1104     1S -0.0632     2V -0.1277    13V  0.2052

Eigenvalues

         -2.0903        -3.4787        -3.9223        -5.3226        -5.8202        -7.2513        -7.7746        -9.2626

Eigenvectors   17            18             19             20             21             22             23             24

     12V -0.6294   18V  0.5559    20V -0.5049    26V  0.5332    28V  0.4399    34V  0.5039    39V  0.4059    42V -0.4927
      7V  0.4915   13V  0.5037    15V  0.4522    23V  0.3905    23V -0.3996    31V  0.4577    29V  0.3795    39V -0.4451
      4V -0.3638   15V  0.3066    23V -0.3489    21V  0.3783    31V  0.3788    44V  0.2923    36V  0.3741    52V -0.2701
     15V -0.2792   20V -0.2667    13V -0.3360    13V  0.2855    21V  0.3479    36V -0.2901    26V  0.3351    45V  0.2639

Eigenvalues

         -9.7908       -11.6594       -12.7869       -14.7634       -47.0364       -72.1774       -78.8232      -100.3271

Eigenvectors   25            26             27             28             29             30             31             32

     47V  0.3812   47V -0.5831    45V  0.4978    55V -0.5524     2V  0.8814     7V -0.6711    10V -0.6328    20V  0.6282
     44V  0.3774   52V  0.4132    50V  0.4640    60V  0.4651     1C -0.3571    12V -0.5613     5V  0.5176    15V  0.5375
     39V -0.3487   50V -0.3304    55V  0.4383    50V  0.3803     7V  0.2965     4C  0.4147     5C  0.4214     8C -0.4549
     34V  0.3392   60V -0.3007    42V  0.3713    47V -0.2864     4V  0.0690     2V  0.2184    15V -0.3686    10V -0.3058

*** LANDAU-LEVELS IN ZINCBLENDE-TYPE SEMICONDUCTORS ***

INSB.DAT


transitions-energies and oscillator strengths

initial states    1 -   7
final states      1 -   7

lower bound  [meV]                                          0.00000
upper bound  [meV]                                         10.00000
minimum oscillator strength considered for transitions :    0.05000


transition  1 --> 1

  INITIAL STATE          FINAL STATE          DIFFERENCE              OSCILLATOR

  n  fct       meV      n  fct       meV        meV         1/cm      parallel

  1  27C    435.24      2  26C    428.47       6.77 .182979E+07        0.1959

  2  26C    428.47      1  27C    435.24       6.77 .182979E+07        0.1959

  3  23C    417.44      4  22C    410.54       6.90 .179562E+07       -0.1185

  4  22C    410.54      3  23C    417.44       6.90 .179562E+07       -0.1185

  5  19C    398.40      6  18C    391.22       7.18 .172546E+07       -0.1159

  6  18C    391.22      5  19C    398.40       7.18 .172546E+07       -0.1159
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