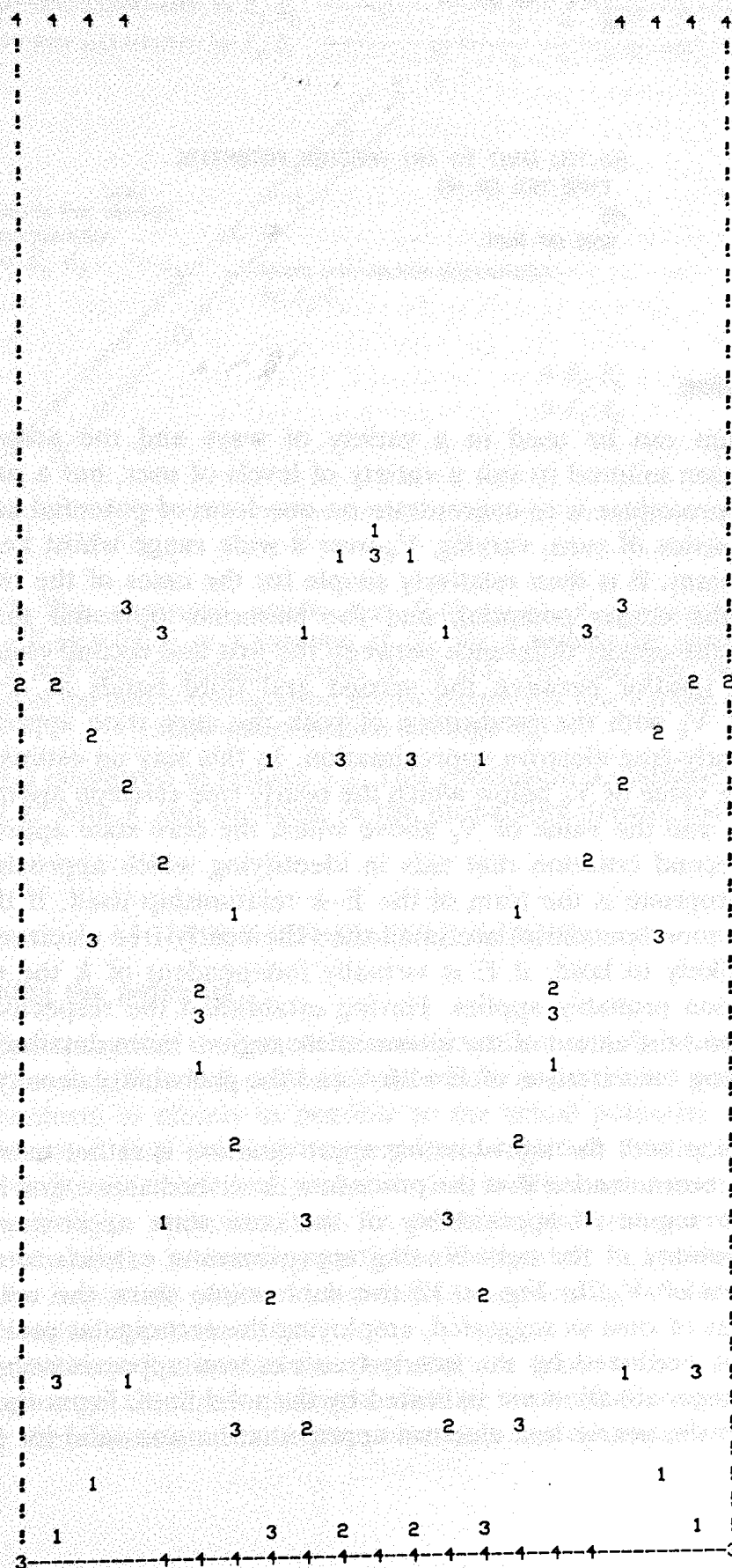PROBABILITY DENSITY VS X FOR FIRST THREE STATES.
THE POTENTIAL IS SHOWN AS 4

```
DO YOU WANT TO CALCULATE ANOTHER SET OF
PROBABILITY DENSITY FUNCTIONS
TYPE YES OR NO
NO
```

```
DO YOU WANT TO TRY ANOTHER POTENTIAL
TYPE YES OR NO
NO
END OF RUN
```

3.2 Discussion

The program can be used in a variety of ways and the accompanying documentation tailored to suit a variety of levels of user, but a particularly instructive procedure is to concentrate on one form of potential and first to perform a series of runs, varying V_0 over a wide range whilst keeping the period constant. It is then relatively simple for the cases of the rectangular potential, the cosine potential, and the harmonic potential to compare graphically the energy difference between the first and second energy bands at $k = \pi/a$ (and/or between the second and third bands at $k = 0$) as a function of V_0 with the predictions of both the core state approximation, and the nearly-free electron approximation. In this way an estimate can be made of the value of V_0 below which the nearly free electron approximation is accurate, and the value of V_0 above which the core state approximation holds. A second criterion that aids in identifying which approximation, if any, is appropriate is the form of the $E-k$ relationship itself. If the energy gaps at the zone boundaries are small then the nearly-free electron approximation is likely to hold; if E is virtually independent of k the core state approximation probably applies. Having established the respective regions of validity and the extent of the intermediate region, more detailed comparisons involving the variation of E with k and the probability density can then be made.

Comparison with the tight-binding approximation is rather more complicated. It is recommended that the procedure described above first be used to identify the region of applicability of the core state approximation; the region of validity of the tight-binding approximation extends to somewhat lower values of V_0. In Figure 12 the data points show the results for a typical series of runs as suggested, employing the rectangular potential. The energy gaps predicted by the nearly-free electron approximation and the core state approximation are indicated by the solid lines. From the graphs it is clear that the nearly-free electron approximation was valid for the choice
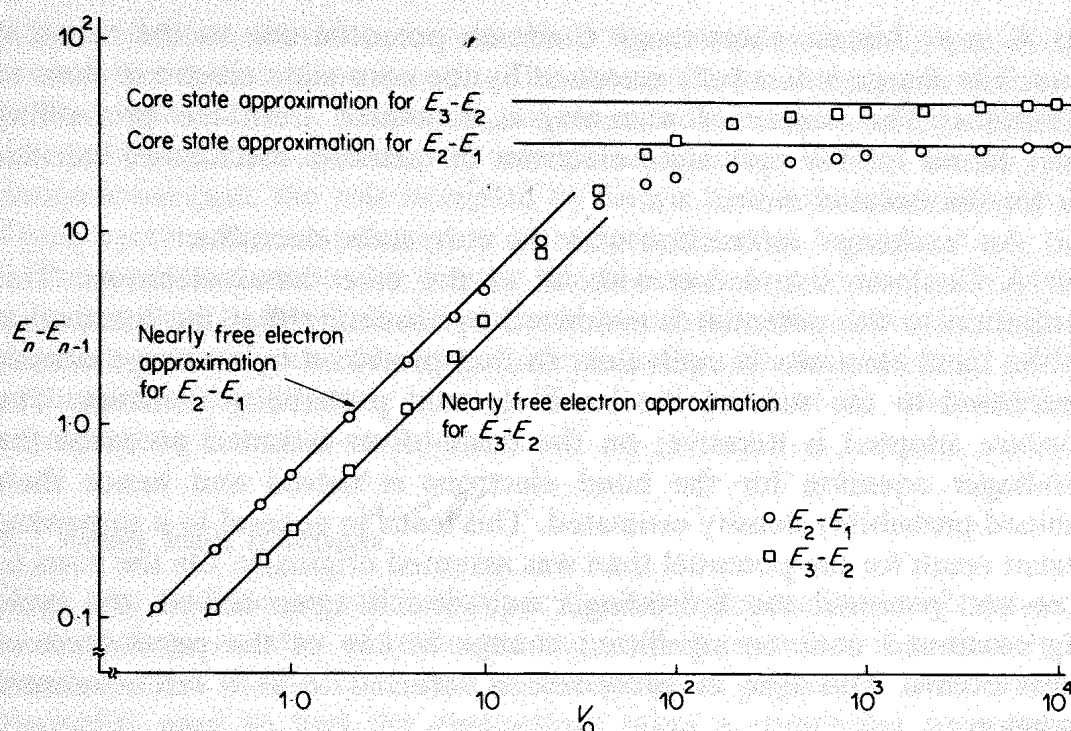
Figure 12. The computed results for $E_2(k = \pi/a) - E_1(k = \pi/a)$(○) and $E_3(k = 0) - E_2(k = 0)$(□) as a function of V_0 for a rectangular potential of period 1.5 and with a rectangle width (b) of 0.5. The solid lines show the predictions of the nearly-free electron approximation (for low V_0) and the core state approximation (for high V_0)

of parameters employed in section 3.2. This conclusion is consistent with the variation of E with k and the form of the probability density found in that case.

4. FURTHER CALCULATIONS

4.1 Estimating the potential

In the present program the potential can be varied widely in form, magnitude, and period. In a full-scale calculation for a particular material it is chosen to conform as closely as possible to the actual potential. It should, however, be noted that treating the problem as that of finding the eigenstates of a single electron in a potential due to the nuclei and the other electrons is itself an approximation. In principle the true wave function should embrace all the interacting particles. Fortunately, it appears that the results for the important physical properties are generally satisfactory using the single-electron approximation.

The principal contributions to the potential are taken to be:

(i) A long-range Coulomb potential due to each of the atomic nuclei screened by their associated core state electrons less the band electrons.

(ii) A more intense short-range Coulomb potential due to the fact that the nuclear charge is less fully screened by the core state electrons close to the nucleus. The degree of screening is estimated from the probability density found for the core state electrons in quantum-mechanical calculations for the isolated atom.

(iii) An 'exchange' interaction with the core state electrons.

(iv) A Coulomb interaction with all of the *other* band electrons. This contribution to the potential is estimated by assuming that the interaction with the band electrons is equivalent to that produced by a charge density proportional to the sum of the band electron probability densities. The procedure adopted is iterative; on the basis of an assumed potential the Schrödinger equation for the band electrons is solved and hence their combined probability density estimated. This leads in general to a somewhat different result for the potential than was assumed originally. On the basis of the revised potential the Schrödinger equation is again solved, the cycle being continued until no significant change in any of the parameters of interest occurs. This type of procedure is referred to as a self-consistent calculation.

4.2 The three-dimensional case

In a normal crystalline conductor the band electrons are free to move in three dimensions. The major difference introduced by this elaboration into the formalism of band calculations is that several quantities which can be treated as scalars in a one-dimensional model have to be recognized as vectors in the three-dimensional case. This is obviously the case for the variable used to represent position in the crystal; x has been used here for the one-dimensional case, $\mathbf{r}$ is generally used in the three-dimensional case. Similarly, the scalar k becomes the vector $\mathbf{k}$. The one-dimensional free electron wave function $\psi(x) = \exp(\mathrm{i}kx)$ becomes $\psi(\mathbf{r}) = \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{r})$ and specifies the value at $\mathbf{r}$ of a wave function of wavelength $\lambda = 2\pi/|\mathbf{k}|$ propagating in the direction of the vector $\mathbf{k}$ (the wave vector). One speaks of 'k-space' or 'reciprocal space' ($\mathbf{k}$ has units L^{-1}).

The quantity corresponding to $2n\pi/a$, which arises as a consequence of Bragg reflections and determines the zone boundaries, must also be expressed as a vector in the three-dimensional case. The condition for Bragg reflection is $2a \sin \theta = n\lambda$ (where a is the spacing between the atomic *planes*), i.e.

$$2a \sin \theta = n\frac{2\pi}{|\mathbf{k}|},$$

so that

$$|\mathbf{k}| \sin \theta = \frac{n\pi}{a}.$$

Bragg reflection therefore occurs when the component of $\mathbf{k}$ in a direction normal to a lattice plane is $n\pi/a$. The change in the component of $\mathbf{k}$ normal to the plane is $2n\pi/a$. Vectors $\mathbf{K}_n$, of magnitude $2n\pi/a$ directed normally to the various lattice planes, of interplane spacing a, fill, in the three-dimensional case, the role occupied by $2n\pi/a$ in the one-dimensional case. These vectors $\mathbf{K}_n$ are referred to as reciprocal lattice vectors.

The most important new feature which occurs as a consequence of these considerations in the three-dimensional case is that the electron energy now depends not only on the magnitude but also on the direction of $\mathbf{k}$. In consequence the effective mass is likewise dependent on direction and is expressed as a second-rank tensor.

4.3 Other basis functions

Since any realistic potential involves Coulomb interactions with the atomic nuclei a large number of terms are required to represent it accurately by a Fourier series of the kind used in the program presented here. Since the algorithm used to find the eigenvalues takes a computing time approximately proportional to the cube of the number of terms employed, this feature can render the accurate solution of the problem completely impracticable. For this reason alternative basis functions are generally used in full-scale band structure calculation. Three of the most widely used approaches are as follows.

(i) The Orthogonalized Plane Wave (OPW) method[11]

The core state electrons are of no real interest in a band structure calculation—their energies and wave functions are already known from calculations on the free atom and are unchanged in the solid. In the method of orthogonalized plane waves the core states are deliberately ignored by using the Schmidt orthogonalization procedure to construct basis functions which consist of a linear combination of plane waves and core states. The basis functions so formed are orthogonal to the core states.

(ii) The Augmented Plane Wave (APW) method[12]

The potential close to an atomic nucleus in a solid is nearly spherically symmetrical about the nucleus; well away from the nuclei it is nearly constant. In the augmented plane wave approach the radial part of the Schrödinger equation in the regions close to the nuclei is solved by numerical integration. The full solutions—the product of the radial solutions and the spherical harmonics—are matched at the surface of non-overlapping spheres, centred on each of the nuclei, to plane waves (plane waves being the solutions to the Schrödinger equation in a region of constant potential).

A set of plane waves, each differing in wave vector by a reciprocal lattice vector and each matched to the solutions close to the nucleus, are used as basis functions for the variational method.

(iii) *The scattering or Korringa, Kohn, and Rostoker (KKR) method*[13]

This method is allied to the phase-shift method used in scattering theory. The basis functions are made up of ingoing and outgoing spherical waves centred on the nuclei. In the most common form of this method the Green's function approach is employed to cast the Schrödinger equation in integral form.

For materials with $Z \geqslant 55$ relativistic corrections become important, and all of these methods can, if necessary, be modified to incorporate these effects.[14-16]

In principle, provided the basis functions form a complete set, the results of a band structure calculation should be independent of the choice of basis functions—provided enough are used. In practice there are always some deviations, though they are usually small.

4.4 Metals and semiconductors

The methods employed in band structure calculations for metals and semiconductors are quite similar; their different physical properties arise because a metal has one or more partially filled bands, a semiconductor at the absolute zero of temperature has energy bands that are either completely full (the valence band and the core states) or completely empty (the conduction band).

In the case of a metal, band structure calculations lead to an estimate of the density of states, the Fermi energy, and hence of the form of the Fermi surface—the energy surface in **k**-space which delineates the boundary between the filled and the empty electron states at the absolute zero. In a metal it is the electrons close to the Fermi surface that are responsible for the electronic transport properties.

In the case of a semiconductor the most important features determined by a band structure calculation are the energy gap between the valence band and the conduction band, the effective masses and the densities of states of the hole states close to the top of the valence band, and the electron states at the bottom of the conduction band. It is these states which lead to electronic conduction in semiconductors.

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ENERGY BANDS

```
C        MASTER SEGMENT OF PROGRAM.
C        THIS SEGMENT CONTAINS SECTIONS WHERE DATA
C        IS INPUT FROM A TERMINAL.
C        CHANGES WOULD BE NECESSARY TO RUN THE PROGRAM
C        IN BATCH MODE.
         DOUBLE PRECISION H(33,33),A(33),E(33),EF(33,33),W(33)
         COMMON AMP,WIDTH,PERIOD,PI,NPOT,FVAL(20),XVAL(20),NVAL
         REAL K,EL(21,3),KX(21),EM(21,3),ELEC(21,3),WF(21,4),XX(21)
         LOGICAL LOG,LOG1,LOG2,LOG3
         DATA YY,YN,EE,EH/4HYES ,4HNO   ,1HE,1HH/
         PI = 4.0*ATAN(1.0)
         WRITE(1,190)
         WRITE(1,191)
         WRITE(1,192)
         WRITE(1,193)
         WRITE(1,194)
       1 WRITE(1,200)
         WRITE(1,201)
         WRITE(1,202)
         WRITE(1,203)
         WRITE(1,204)
         WRITE(1,205)
         READ(1,100)NPOT
         IF(NPOT.EQ.1) GOTO 10
         IF(NPOT.EQ.2) GOTO 20
         IF(NPOT.EQ.3) GOTO 30
         IF(NPOT.EQ.4) GOTO 40
         IF(NPOT.EQ.5) GOTO 50
         WRITE(1,207)
         GOTO 1
C        DATA FOR RECTANGULAR POTENTIAL
      10 WRITE(1,210)
         WRITE(1,211)
         READ(1,101) AMP
         WRITE(1,212)
         READ(1,101) WIDTH
         WRITE(1,208)
         READ(1,101) PERIOD
         IF(PERIOD.GT.WIDTH) GOTO 70
         WRITE(1,213)
         GOTO 10
C        DATA FOR SAWTOOTH POTENTIAL
      20 WRITE(1,220)
         WRITE(1,221)
         READ(1,101)AMP
         WRITE(1,208)
         READ(1,101)PERIOD
         GOTO 70
C        DATA FOR COSINE POTENTIAL
      30 WRITE(1,230)
         WRITE(1,231)
         WRITE(1,241)
         READ(1,101)AMP
         WRITE(1,208)
         READ(1,101)PERIOD
         GOTO 70
```

ENERGY BANDS

```
C         DATA FOR HARMONIC POTENTIAL
   40 WRITE(1,240)
      WRITE(1,241)
      READ(1,101)AMP
      WRITE(1,208)
      READ(1,101)PERIOD
      AMP=AMP*4.0/(PERIOD*PERIOD)
      GOTO 70
C         DATA FOR INTERPOLATED POTENTIAL
   50 WRITE(1,250)
      WRITE(1,251)
      WRITE(1,252)
      WRITE(1,253)
   51 WRITE(1,271)
      WRITE(1,256)
      READ(1,102)NVAL
      IF(NVAL.LT.2) GOTO 51
      IF(NVAL.GT.20) GOTO 51
   52 WRITE(1,257)
      READ(1,101)FVAL(1)
      XVAL(1)=0.0
      DO 54 I=2,NVAL
      WRITE(1,258)
      READ(1,101)XVAL(I)
      IF(XVAL(I).GT.XVAL(I-1)) GOTO 53
      WRITE(1,270)
      GOTO 52
   53 WRITE(1,259)
      READ(1,101)FVAL(1)
   54 CONTINUE
      PERIOD=2.0*XVAL(NVAL)
      GOTO 70
   70 NPTS=100.0*PERIOD
C         CALCULATION OF RESULTS FOR E-K DIAGRAM
      CALL FRANCS(33,NPTS,DC,A)
      WRITE(1,300)PERIOD
      WRITE(1,301)
      DO 2 L=1,21
      K=0.05*PI*FLOAT(L-1)/PERIOD
      LOG=.FALSE.
      IF(L.LE.10)NAR=10
      IF(L.GT.10)NAR=11
   12 CONTINUE
      CALL ENERGY(K,E,EF,NAR,NAR,DC,A,H,W,.TRUE.)
      IF(LOG)GOTO 13
      E1=E(1)
      E2=E(2)
      E3=E(3)
      NAR=NAR+2
      LOG=.TRUE.
      GOTO 12
   13 CONTINUE
      F1=E(1)
      F2=E(2)
      F3=E(3)
      LOG=.FALSE.
```

ENERGY BANDS

```
      DE=F3-F1
      IF(DE.EQ.0.0)DE=F3
      NAR=NAR+8
      LOG1=.TRUE.
      LOG2=.TRUE.
      LOG3=.TRUE.
      ERES=ABS((F1-E1)/DE)
      IF(ERES.GT.3.0E-3)LOG1=.FALSE.
      ERES=ABS((F2-E2)/DE)
      IF(ERES.GT.3.0E-?)LOG2=.FALSE.
      ERES=ABS((F3-E3)/DE)
      IF(ERES.GT.3.0E-3)LOG3=.FALSE.
      IF(LOG1.AND.LOG2.AND.LOG3)GOTO 16
      IF(NAR.LE.31)GOTO 12
C   OUTPUT WARNING IF ONE OF THE ACCURACIES IS BELOW LIMITS
      IF(.NOT.LOG1.AND.LOG2.AND.LOG3)WRITE(1,400)
  400 FORMAT(41H *** WARNING ACCURACY OF E1 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF(LOG1.AND.(.NOT.LOG2).AND.LOG3)WRITE(1,401)
  401 FORMAT(41H *** WARNING ACCURACY OF E2 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF(LOG1.AND.LOG2.AND.(.NOT.LOG3))WRITE(1,402)
  402 FORMAT(41H *** WARNING ACCURACY OF E3 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF((.NOT.LOG1).AND.(.NOT.LOG2).AND.LOG3)WRITE(1,403)
  403 FORMAT(48H *** WARNING ACCURACY OF E1 AND E2 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF((.NOT.LOG1).AND.LOG2.AND.(.NOT.LOG3))WRITE(1,404)
  404 FORMAT(48H *** WARNING ACCURACY OF E1 AND E3 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF(LOG1.AND.(.NOT.LOG2).AND.(.NOT.LOG3))WRITE(1,405)
  405 FORMAT(48H *** WARNING ACCURACY OF E2 AND E3 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
      IF((.NOT.LOG1).AND.(.NOT.LOG2).AND.(.NOT.LOG3))WRITE(1,406)
  406 FORMAT(52H *** WARNING ACCURACY OF E1, E2 AND E3 ON NEXT LINE ,
     1 13HUNCERTAIN ***)
   16 CONTINUE
      KX(L)=K
      DO 3 N=1,3
      EL(L,N)=E(N)
    3 CONTINUE
      WRITE(1,302) KX(L),(EL(L,N),N=1,3)
    2 CONTINUE
    4 WRITE(1,280)
      WRITE(1,291)
      READ(1,103) YA
      IF(YA.EQ.YN) GOTO 5
      IF(YA.NE.YY) GOTO 4
      WRITE(1,303)
      CALL GRAPH(EL,21,3,KX)
    5 WRITE(1,281)
      WRITE(1,291)
      READ(1,103) YA
      IF(YA.EQ.YN) GOTO 71
      IF(YA.NE.YY) GOTO 5
      WRITE(1,304)
```

ENERGY BANDS

```
      WRITE(1,305)
C        APPROXIMATE CALCULATION OF EFFECTIVE MASS
C        THE VALUE IS TRUNCATED AT 10**6 TIMES THE
C        MASS OF A FREE ELECTRON
      DK2=(KX(2)-KX(1))**2
      DO 7 N=1,3
      EM(1,N)=2.0*(EL(2,N)-EL(1,N))/DK2
      DO 6 L=2,20
      EM(L,N)=(EL(L+1,N)+EL(L-1,N)-2.0*EL(L,N))/DK2
    6 CONTINUE
      EM(21,N)=2.0*(EL(20,N)-EL(21,N))/DK2
    7 CONTINUE
      DO 8 L=1,21
      DO 9 N=1,3
      IF(EM(L,N).GE.0.0) ELEC(L,N)=EE
      IF(EM(L,N).LT.0.0) ELEC(L,N)=EH
      IF(ABS(EM(L,N)).GT.2.0E-6) GOTO 80
      EM(L,N)=2.0E-6
   80 EM(L,N)=2.0/ABS(EM(L,N))
    9 CONTINUE
      WRITE(1,310) KX(L),(EM(L,N),ELEC(L,N),N=1,3)
    8 CONTINUE
   81 WRITE(1,280)
      WRITE(1,291)
      READ(1,103) YA
      IF(YA.EQ.YN) GOTO 71
      IF(YA.NE.YY) GOTO 81
      WRITE(1,306)
      DO 82 L=1,21
      DO 82 N=1,3
      IF(EM(L,N).GT.50.0) EM(L,N)=50.0
   82 CONTINUE
      CALL GRAPH(EM,21,3,KX)
   71 WRITE(1,282)
      WRITE(1,283)
      WRITE(1,291)
      READ(1,103) YA
      IF(YA.EQ.YN) GOTO 78
      IF(YA.NE.YY) GOTO 71
   72 WRITE(1,284)
      READ(1,101) K
C        CALCULATION OF PROBABILITY DENSITY FUNCTIONS
      CALL ENERGY(K,E,EF,15,15,DC,A,H,W,.FALSE.)
      DO 73 I=1,21
      XX(I)=0.05*FLOAT(I-11)*PERIOD
      X=XX(I)
      WF(I,4)=V(X)
      DO 74 J=1,3
      WF(I,J)=PROB(J,EF,15,15,X)
   74 CONTINUE
   73 CONTINUE
      WRITE(1,307)
      DO 75 I=1,21
      WRITE(1,302) XX(I),(WF(I,J),J=1,4)
   75 CONTINUE
   76 WRITE(1,280)
```

ENERGY BANDS

```
        WRITE(1,291)
        READ(1,103) YA
        IF(YA.EQ.YN) GOTO 77
        IF(YA.NE.YY) GOTO 76
        WRITE(1,308)
        WRITE(1,309)
        PDMAX=WF(1,1)
        DO 771 I=1,21
        DO 771 J=1,3
        IF(WF(I,J).GT.PDMAX) PDMAX=WF(I,J)
  771 CONTINUE
        VMAX=ABS(WF(1,4))
        DO 772 I=2,21
        IF(ABS(WF(I,4)).GT.VMAX) VMAX=ABS(WF(I,4))
  772 CONTINUE
        IF(VMAX.LT.0.1*PDMAX) VMAX=0.5*PDMAX
        SCALE=1.5*PDMAX/VMAX
        DO 773 I=1,21
        WF(I,4)=WF(I,4)*SCALE
  773 CONTINUE
        CALL GRAPH(WF,21,4,XX)
   77 WRITE(1,285)
        WRITE(1,286)
        WRITE(1,291)
        READ(1,103) YA
        IF(YA.EQ.YN) GOTO 78
        IF(YA.NE.YY) GOTO 77
        GOTO 72
   78 WRITE(1,290)
        WRITE(1,291)
        READ(1,103) YA
        IF(YA.EQ.YN) GOTO 90
        IF(YA.NE.YY) GOTO 78
        GOTO 1
   90 WRITE(1,299)
        STOP
C     FORMATS FOR INTERACTIVE SECTIONS OF PROGRAM.
  100 FORMAT(I1)
  101 FORMAT(F10.4)
  102 FORMAT(I2)
  103 FORMAT(A4)
  190 FORMAT(1X,49HPROGRAM TO CALCULATE FIRST THREE ENERGY LEVELS OF)
  191 FORMAT(1X,50HAN ELECTRON SUBJECT TO A GIVEN PERIODIC POTENTIAL.)
  192 FORMAT(1X,39HALL INPUT AND OUTPUT IS IN ATOMIC UNITS)
  193 FORMAT(1X,44HI.E. THE UNIT OF DISTANCE IS ONE BOHR RADIUS)
  194 FORMAT(1X,33HTHE UNIT OF ENERGY IS ONE RYDBERG//)
  200 FORMAT(1X,34HWHAT SORT OF POTENTIAL DO YOU WANT)
  201 FORMAT(1X,32HTYPE 1 FOR RECTANGULAR POTENTIAL)
  202 FORMAT(1X,29HTYPE 2 FOR SAWTOOTH POTENTIAL)
  203 FORMAT(1X,27HTYPE 3 FOR COSINE POTENTIAL)
  204 FORMAT(1X,29HTYPE 4 FOR HARMONIC POTENTIAL)
  205 FORMAT(1X,33HTYPE 5 FOR INTERPOLATED POTENTIAL)
  207 FORMAT(1X,36HNUMBER INPUT MUST BE BETWEEN 1 AND 5)
  208 FORMAT(1X,27HINPUT PERIOD AS PEAL NUMBER)
  210 FORMAT(1X,21HRECTANGULAR POTENTIAL)
  211 FORMAT(1X,40HINPUT HEIGHT OF RECTANGLE AS REAL NUMBER)
```

ENERGY BANDS

```
  212 FORMAT(1X,39HINPUT WIDTH OF RECTANGLE AS REAL NUMBER)
  213 FORMAT(1X,46HPERIOD MUST BE GREATER THAN WIDTH OF RECTANGLE)
  220 FORMAT(1X,18HSAWTOOTH POTENTIAL)
  221 FORMAT(1X,39HINPUT HEIGHT OF SAWTOOTH AS REAL NUMBER)
  230 FORMAT(1X,37HCOSINE POTENTIAL I.E. PROPORTIONAL TO)
  231 FORMAT(1X,24H1.0-COS(2.0*PI*X/PERIOD))
  240 FORMAT(1X,49HHARMONIC POTENTIAL I.E. PROPORTIONAL TO X SQUARED)
  241 FORMAT(1X,48HINPUT CONSTANT OF PROPORTIONALITY AS REAL NUMBER)
  250 FORMAT(1X,22HINTERPOLATED POTENTIAL)
  251 FORMAT(1X,46HTHE POTENTIAL IS GIVEN BY LINEAR INTERPOLATION)
  252 FORMAT(1X,44HBETWEEN POINTS SPECIFIED OVER HALF A PERIOD.)
  253 FORMAT(1X,38HTHE PERIOD IS TWICE THE FINAL X VALUE.)
  256 FORMAT(1X,22HINPUT NUMBER OF POINTS)
  257 FORMAT(1X,43HINPUT AS REAL NUMBER THE POTENTIAL AT X=0.0)
  258 FORMAT(1X,33HINPUT NEXT X VALUE AS REAL NUMBER)
  259 FORMAT(1X,30HINPUT POTENTIAL AS REAL NUMBER)
  270 FORMAT(1X,42HEACH X VALUE MUST BE GREATEP THAN LAST ONE)
  271 FORMAT(1X,46HTHE NUMBER OF POINTS MUST BE BETWEEN 02 AND 20)
  280 FORMAT(//33HDO YOU WANT TO PLOT THESE RESULTS)
  281 FORMAT(//43HDO YOU WANT TO CALCULATE THE EFFECTIVE MASS)
  282 FORMAT(//48HDO YOU WANT TO CALCULATE THE PROBABILITY DENSITY)
  283 FORMAT(1X,43HFUNCTIONS FOR THE FIRST THPEE ENERGY STATES)
  284 FORMAT(1X,35HINPUT A VALUE OF K AS A REAL NUMBER)
  285 FORMAT(1X,39HDO YOU WANT TO CALCULATE ANOTHER SET OF)
  286 FORMAT(1X,29HPROBABILITY DENSITY FUNCTIONS)
  290 FORMAT(////36HDO YOU WANT TO TRY ANOTHER POTENTIAL)
  291 FORMAT(1X,14HTYPE YES OR NO)
  299 FORMAT(1X,10HEND OF RUN)
C     *****************************************************
  300 FORMAT(//6X,6HPERIOD,F12.1)
  301 FORMAT(/7X,1HK,9X,2HE1,8X,2HE2,8X,2HE3)
  302 FORMAT(1X,5F10.4)
  303 FORMAT(//5X,45HE-K DIAGRAM SHOWING FIRST THREE ENERGY LEVELS//)
  304 FORMAT(//34HTHE MASS OF A FREE ELECTRON IS 1.0)
  305 FORMAT(//7X,1HK,10X,2HM1,9X,2HM2,9X,2HM3)
  306 FORMAT(//5X,45HABS(EFFECTIVE MASS) VS K IN FIRST THREE BANDS)
  307 FORMAT(//7X,1HX,9X,3HPD1,7X,3HPD2,7X,3HPD3,7X,1HV)
  308 FORMAT(//5X,48HPROBABILITY DENSITY VS X FOR FIRST THREE STATES.)
  309 FORMAT(1X,27HTHE POTENTIAL IS SHOWN AS 4//)
  310 FORMAT(1X,F10.4,3(F9.2,1X,A1))
      END
C
      SUBROUTINE ENERGY(K,E,EV,ND,N,DC,A,H,W,BOOL)
C
C        SUBROUTINE TO CALCULATE THE FIRST N ENERGY LEVELS
C·       AND CORRESPONDING STATE VECTORS FOR GIVEN K AND
C        GIVEN PERIODIC POTENTIAL.
C        F02ABF IS A NAG LIBRARY ROUTINE THAT CALCULATES
C        THE EIGENVALUES AND EIGENVECTORS OF A REAL
C        SYMMETRIC MATRIX.
C        F02AAF IS A NAG LIBRARY ROUTINE THAT CALCULATES
C        JUST THE EIGENVALUES OF A REAL SYMMETRIC MATRIX.
C
      DOUBLE PRECISION E(N),H(ND,N),A(N),EV(ND,N),W(N)
      LOGICAL BOOL
      COMMON AMP,WIDTH,PERIOD,PI,NPOT,FVAL(20),XVAL(20),NVAL
```

ENERGY BANDS

```
      REAL K
      N1=N/2
      IF(2*N1.EQ.N) GOTO 1
      N2=(N+1)/2
      DO 2 I=1,N
      H(I,I)=(K-FLOAT(N2-I)*2.0*PI/PERIOD)**2+DC
    2 CONTINUE
      GOTO 3
    1 DO 4 I=1,N
      H(I,I)=(K-FLOAT(N1-I+1)*2.0*PI/PERIOD)**2+DC
    4 CONTINUE
    3 NM=N-1
      DO 5 I=1,NM
      IP=I+1
      DO 5 J=IP,N
      JMI=J-I
      H(I,J)=A(JMI)/2.0
      H(J,I)=H(I,J)
    5 CONTINUE
      IFAIL=0
      IF(BOOL)CALL F02AAF(H,ND,N,E,W,IFAIL)
      IF(.NOT.BOOL)CALL F02ABF(H,ND,N,E,EV,ND,W,IFAIL)
      RETURN
      END
C
      SUBROUTINE FRANCS(NTERMS,NDATA,DC,A)
C
C        SUBROUTINE TO FOURIER ANALYSE THE POTENTIAL.
C        FOR THE INTERPOLATED POTENTIAL THE COEFFICIENTS
C        ARE EVALUATED BY NUMERICAL INTEGRATION.
C        FOR THE OTHER POTENTIALS ANALYTIC EXPRESSIONS
C        FOR THE FOURIER COEFFICIENTS ARE USED.
C
      DOUBLE PRECISION A(NTERMS)
      COMMON AMP,WIDTH,PERIOD,PI,NPOT,FVAL(20),XVAL(20),NVAL
      REAL K
      IF(NPOT.EQ.1) GOTO 10
      IF(NPOT.EQ.2) GOTO 20
      IF(NPOT.EQ.3) GOTO 30
      IF(NPOT.EQ.4) GOTO 40
      GOTO 50
C        FOURIER COEFFICIENTS FOR RECTANGULAR POTENTIAL
   10 DC=WIDTH*AMP/PERIOD
      DO 11 M=1,NTERMS
      FM=M
      A(M)=2.0*COS(FM*PI)*AMP*SIN(FM*PI*WIDTH/PERIOD)/(FM*PI)
   11 CONTINUE
      RETURN
C        FOURIER COEFFICIENTS FOR SAWTOOTH POTENTIAL
   20 DC=AMP/2.0
      DO 21 M=1,NTERMS
      FM=M
      A(M)=2.0*AMP*(COS(FM*PI)-1.0)/(FM*PI)**2
   21 CONTINUE
      RETURN
C        FOURIER COEFFICIENTS FOR COSINE POTENTIAL
```

ENERGY BANDS

```
   30 DC=AMP
      A(1)=-AMP
      DO 31 M=2,NTERMS
      A(M)=0.0
   31 CONTINUE
      RETURN
C        FOURIER COEFFICIENTS FOR HARMONIC POTENTIAL
   40 DC=AMP*PERIOD**2/12.0
      DO 41 M=1,NTERMS
      FM=M
      A(M)=AMP*PERIOD**2*COS(FM*PI)/(FM*PI)**2
   41 CONTINUE
      RETURN
C        FOURIER COEFFICIENTS BY NUMERICAL INTEGRATION
   50 K=2.0*PI/PERIOD
      FD=NDATA
      STEP=PERIOD/FD
      DC=V(0.0)
      DO 51 M=1,NTERMS
      A(M)=V(0.0)
   51 CONTINUE
      ND1=NDATA-1
      DO 52 I=1,ND1
      FI=I
      X=FI*STEP
      VX=V(X)
      DC=DC+VX
      DO 53 M=1,NTERMS
      FM=M
      A(M)=A(M)+COS(FM*K*X)*VX
   53 CONTINUE
   52 CONTINUE
      DC=DC/FD
      DO 54 M=1,NTERMS
      A(M)=A(M)*2.0/FD
   54 CONTINUE
      RETURN
      END
C
      FUNCTION V(Y)
C
C        FUNCTION TO EVALUATE THE POTENTIAL AT ANY POINT.
C        THE POTENTIAL IS ALWAYS AN EVEN FUNCTION.
C
      COMMON AMP,WIDTH,PERIOD,PI,NPOT,FVAL(20),XVAL(20),NVAL
      X=Y
      IF(X.LT.0.0) X=-X
      P2=PERIOD/2.0
      R=AMOD(X,PERIOD)
      IF(R.GT.P2) R=PERIOD-R
      IF(NPOT.EQ.1) GOTO 10
      IF(NPOT.EQ.2) GOTO 20
      IF(NPOT.EQ.3) GOTO 30
      IF(NPOT.EQ.4) GOTO 40
      GOTO 50
C        RECTANGULAR POTENTIAL
```

ENERGY BANDS

```
   10 B=(PERIOD-WIDTH)/2.0
      IF(R.LT.B) V=0.0
      IF(R.EQ.B) V=AMP/2.0
      IF(R.GT.B) V=AMP
      RETURN
C        SAWTOOTH POTENTIAL
   20 V=R*AMP/P2
      RETURN
C        COSINE POTENTIAL
   30 Q=2.0*PI/PERIOD
      V=AMP*(1.0-COS(Q*R))
      RETURN
C        HARMONIC POTENTIAL
   40 V=AMP*R**2
      RETURN
C        INTERPOLATED POTENTIAL
   50 NV1=NVAL-1
      DO 51 I=1,NV1
      IF(R.GE.XVAL(I).AND.R.LT.XVAL(I+1)) J=I
   51 CONTINUE
      GRAD=(FVAL(J+1)-FVAL(J))/(XVAL(J+1)-XVAL(J))
      V=FVAL(J)+GRAD*(R-XVAL(J))
      RETURN
      END
C
      FUNCTION PROB(L,EV,ND,N,X)
C
C     FUNCTION TO EVALUATE THE PROBABILITY DENSITY AT X
C     FOR GIVEN K AND GIVEN STATE VECTOR.
C
      DOUBLE PRECISION EV(ND,N)
      COMMON AMP,WIDTH,PERIOD,PI,NPOT,FVAL(20),XVAL(20),NVAL
      S=0.0
      ND1=ND-1
      DO 1 I=1,ND1
      I1=I+1
      DO 2 J=I1,ND
      F=2.0*PI*FLOAT(J-I)/PERIOD
      S=S+EV(I,L)*EV(J,L)*COS(F*X)
    2 CONTINUE
    1 CONTINUE
      PROB=1.0+2.0*S
      RETURN
      END
C
      SUBROUTINE GRAPH(Y,NP,NG,X)
C
C     SUBROUTINE TO PLOT UP TO FOUR FUCTIONS
C     ON THE SAME GRAPH.
C
      DIMENSION Y(NP,NG),X(NP),PLOT(120),PLT(7)
      DATA PLT(1),PLT(2),PLT(3),PLT(4),PLT(5),PLT(6),PLT(7)/
     1 4H1   ,4H2   ,4H3   ,4H4   ,4H    ,4H-   ,4H!   /
      IWG=70
      GAP=FLOAT(IWG-1)/FLOAT(NP-1)
      IGAP=IFIX(AINT(GAP))
```

ENERGY BANDS

```
      IWG=(NP-1)*IGAP+1
      YMIN=Y(1,1)
      YMAX=Y(1,1)
      DO 66 N=1,NG
      DO 68 I=1,NP
      IF(Y(I,N).LT.YMIN) YMIN=Y(I,N)
      IF(Y(I,N).GT.YMAX) YMAX=Y(I,N)
   68 CONTINUE
   66 CONTINUE
      IF(YMIN.GT.0.0) YMIN=0.0
      IHG=IWG
      SCALE=(YMAX-YMIN)/FLOAT(IHG-1)
      DO 70 J=1,IHG
      YTS=YMAX-SCALE*(FLOAT(J)-1.5)
      YBS=YMAX-SCALE*(FLOAT(J)-0.5)
      PLOT(1)=PLT(7)
      PLOT(IWG)=PLT(7)
      DO 72 I=1,NP
      K1=(I-1)*IGAP+1
      K2=I*IGAP
      DO 74 K=K1,K2
      IF(K.NE.1.AND.K.NE.IWG) PLOT(K)=PLT(5)
      IF(YTS.GE.0.0.AND.YBS.LT.0.0) PLOT(K)=PLT(6)
   74 CONTINUE
      DO 73 N=1,NG
      IF(Y(I,N).LE.YTS.AND.Y(I,N).GT.YBS) PLOT(K1)=PLT(N)
   73 CONTINUE
   72 CONTINUE
      WRITE(1,178)(PLOT(K),K=1,IWG)
  178 FORMAT(1H ,120A1)
   70 CONTINUE
   62 CONTINUE
      RETURN
      END
```

PART 4

Applied Physics

CHAPTER 11

Computer Simulation of Hot Electron Behaviour in Semiconductors Using Monte Carlo Methods

A. D. BOARDMAN

1. INTRODUCTION

Transistors become less effective as the operation frequency increases. This is particularly true in the microwave (GHz) range of frequencies. This fact has stimulated, for many years, a great deal of research effort directed towards the development of devices that behave as microwave sources or act as microwave amplifiers.

In 1963, Gunn[1] discovered that the current through bulk gallium arsenide (GaAs) becomes unstable and fluctuates periodically at a microwave frequency, provided the applied bias field (cf. Figure 1) exceeds a certain critical value, thus confirming earlier theoretical work by Ridley and Watkins[2] and Hilsum.[3] It is now known as the Gunn effect. The word 'bulk' is significant because, in the bulk device shown in Figure 1, there are no gates or junctions. Instead of the electrons becoming warm, as they do in a normal transistor, they become hot and then use the peculiarities of the band structure to transfer from one part of momentum space to another.

For materials in which such transfers can take place, such as GaAs, the low field behaviour fits the familiar Ohm's law, but at strong electric fields a deviation from Ohm's law occurs. Therefore, in the variation of mean velocity v, against electric field F, as sketched in Figure 2, the differential mobility dv/dF is negative beyond a field value called the threshold bias. A simple argument shows that it is this possibility of voltage-controlled negative resistance in the bulk that leads to instability and hence to microwave current oscillations.

Consider the one-dimensional forms of the equation of continuity and