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A COMPUTER PROGRAM TO CALCULATE SYNCHROTRON RADIATION SPECTRA

by

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1. INTRODUCTION

A program to calculate the synchrotron radiation spectrum of the 5 GeV electron synchrotron NINA is described in this report. The program was written to generate source tables of the radiation spectrum[1] and for use in the investigation of the properties of a diamond crystal detector[2]. The program has since been modified to generate similar spectra for the 2 GeV storage ring of the Synchrotron Radiation Source[3].

The original program differs from other programs written for accelerators in that it allows for the correct variation of energy during the acceleration cycle in the synchrotron.

The spectrum is calculated for the vertical distribution of the polarised components in the wavelength range 0.1 Å to 100,000 Å, at operating energies of 1, 2, 3, 4 and 5 GeV.

The method of calculation and the approximations used for evaluations of the Bessel Functions are discussed. Flow charts for the program are also included.

2. THEORY

The general theory of synchrotron radiation as stated by Schwinger[4] gives the power radiated by an electron per unit wavelength (centred at λ), per radian vertically, at a vertical angle of ψ as

$$P(\psi,\lambda) = \frac{3}{4\pi^2}\,\frac{e^2}{R}\left(\frac{\lambda_c}{\lambda}\right)^2\left(\frac{2\pi c}{\lambda^2}\right)\left(\frac{E}{m_0c^2}\right)^2\left[1+\left(\frac{E\psi}{m_0c^2}\right)^2\right]^2 \times\left[K^2_{2/3}(\epsilon)+\frac{(E\psi/m_0c^2)^2}{1+(E\psi/m_0c^2)^2}\cdot K^2_{1/3}(\epsilon)\right] \qquad (2.1)$$

where $\epsilon = \frac{\lambda_c}{2\lambda}\left[1+\left(\frac{E\psi}{m_0c^2}\right)^2\right]^{3/2}$

- e = electronic charge (e.s.u.)
- R = orbit radius (cm)
- λ = wavelength (cm)
- λ_c = "characteristic wavelength" (cm)
- c = velocity of light (cm.s^{-1})
- E = electron energy } in the same units
- m_0c^2 = electron rest mass } in the same units
- ψ = elevation angle between direction of emission and the orbit plane
- $K_{1/3}$, $K_{2/3}$ = second order Bessel Functions.

In this form the expression is not suited to calculating the desired spectra and when translated into S.I. units it becomes

$$N(\psi,\lambda,E) = \frac{8\pi R^2 e}{h\lambda^2}\,10^{16}\left(\frac{m_0c^2}{E}\right)^4\left(1+\left(\frac{E\psi}{m_0c^2}\right)^2\right)^2 \left[K^2_{2/3}(\epsilon)+\frac{(E\psi/m_0c^2)^2}{1+(E\psi/m_0c^2)^2}\cdot K^2_{1/3}(\epsilon)\right] \qquad (2.2)$$

where $N(\psi,\lambda,E)$ is the number of photons per mA of circulating beam, per mrad horizontally, per mrad vertically, per second, emitted within a 0.1% bandwidth. The units are as follows:

E, m_0c^2	GeV	
ψ	Radians	
R	Metres	
e	Coulomb	
h	Joule.s	(Planck's Constant)
λ	Å	

Knowing the variation of energy with time it is possible to integrate over the acceleration cycle and produce a matrix N which contains the spectrum for the range of ψ and λ.

The two terms inside the square bracket in eqn.(2.2) refer to the parallel and perpendicularly polarised components. The perpendicular component is given by deleting the $K^2_{2/3}(\epsilon)$ term. The program was run twice calculating firstly the parallel polarised component for all five operating energies and secondly the total spectrum for these energies. In subsequent analysis the subtraction of the parallel component from the total was used to compute the perpendicularly polarised spectrum.

3. THE PROGRAM

The problem may be divided into a number of blocks as may be seen from fig.1, the flow chart for the whole program. Each of these blocks is discussed in the following sections.

The wavelength range was from 0.1 Å to 100,000 Å and was put on a logarithmic scale. The wavelength increment was one tenth of a decade so that the full range was covered at 61 points.

The vertical distribution was calculated at 60 points, from the orbit plane (0 mrad) to 10 mrad above this. The range from 0 to 1 mrad was at 0.02 mrad steps and from there to 10 mrad in 1 mrad steps.

Five operating energies were chosen at 1, 2, 3, 4 and 5 GeV, these being representative of the most common in use.

3.1 Energy Variation in NINA

The energy variation is defined by the equation

$$E(t) = E_{max} + \theta/2\ (\sin\ (2\pi\ f\ t - \pi/2) - 1) \qquad (3.1)$$

where t = time (s)

f = accelerating frequency (Hz)

$E(t)$ = energy at time (t) (MeV)

E_{max} = operating energy of the machine (MeV)

There are several conditions of operation which are fixed and which give the following relationships:

$E(t_{inj})$ = 43.0 MeV

where t_{inj} = time at injection into the synchrotron

$\left(\frac{dE}{dt}\right)_{inj}$ = 2.5×10^5 MeV.s^{-1}

Thus

$$t_{inj} = \frac{2\tan^{-1}\left(\frac{1+k}{1-k}\right) + \pi/2}{2\pi\ f} \qquad (3.2)$$

where

$$k = \frac{2\pi\ f\ (43.0 - E_{max})}{2.5 \times 10^5}$$

and

$$\theta = \frac{2.5 \times 10^5}{\pi\ f\ \cos\ (2\pi\ f\ t_{inj} - \pi/2)} \qquad (3.3)$$

For each operating energy the program computes the time at injection using eqn.(3.2) and then the energy at any time during the acceleration cycle may be computed.

3.2 The Bessel Functions

The major part of the computing time is taken up with the evaluation of the Bessel Functions. To cover the argument range two series approximations are used and the transition point between the two is chosen to make the change as smooth as possible.

The relationship:

$$K_n(\epsilon) = \frac{n!\ (-n)!}{2n} \sum_{k=0}^{40} \frac{(\epsilon/2)^{2k-n}}{k!\ (k-n)!} - \frac{(\epsilon/2)^{2k+n}}{k!\ (k+n)!} \qquad (3.4)$$

is used when $\epsilon \le 3.5$. The factorials are computed by using the library function subroutine DGAMMA (which computes Gamma functions in double precision) and using the relationship

$$\Gamma(n) = (n-1)!$$

The range of factorials to be computed is from (-2/3)! to (40 2/3)! in steps of 1/3 and the values are stored in a unidimensional array. The values are accessed using the factorial argument times three as a pointer to the location within this array.

Using the fact that

$$\Gamma(n)\ \Gamma(1-n) = \frac{\pi}{\sin n\pi} \qquad (3.5)$$

eqn.(3.4) reduces to

$$K_n(\varepsilon) = \frac{\pi}{\sqrt{3}} \sum_{k=0}^{40} \frac{(\varepsilon/2)^{2k-n}}{k!\ (k-n)!} - \frac{(\varepsilon/2)^{2k+n}}{k!\ (k+n)!} \qquad (3.6)$$

The series is infinite but it has been shown by other authors[5,6] that it is quite acceptable to sum to 40 terms. The two terms within the summation are evaluated in double precision in order to maintain accuracy when they are large and the difference is small.

The summation is done within a loop and continues to the maximum of 40 terms unless the values become negligibly small, in which case the loop is terminated.

For $\varepsilon > 3.5$ the following expression is used:

$$K_n(\varepsilon) = \left(\frac{\pi}{2\varepsilon}\right)^{1/2} e^{-\varepsilon}\left[1 + \frac{(4n^2-1^2)}{1!\ 8\varepsilon} + \frac{(4n^2-1^2)(4n^2-3^2)}{2!\ (8\varepsilon)^2} \ldots\right] \qquad (3.7)$$

This is initially convergent but becomes divergent in higher order terms. The summation loop is therefore terminated either when the terms are insignificant, when convergence ends, or at the maximum of 40 terms, whichever occurs first.

There is a slight discontinuity at the change from using eqn.(3.6) to eqn.(3.7) but it does not generate any large errors. Equation (3.7) is used for $3.5 < \varepsilon < 15.0$ and for larger arguments the Bessel Functions are set to zero since their contribution to any spectrum is negligibly small – $K_{1/3}(15) \sim 10^{-7}$.

3.3 Integration over the Acceleration Cycle

As was explained in section 3.1 it is possible to calculate the energy at any time during the acceleration cycle once eqn.(3.2) has been solved. The energy is calculated at about 50 times during acceleration at 0.2 ms increments from the time of injection to 11 ms after minimum field. This end point is the normal time at which the radio frequency accelerating field is switched off in the synchrotron.

The spectrum for all ψ and λ is calculated for each energy and the contributions from these are summed to give the total for the biased-sinusoidal energy variation, as a spectrum time averaged over one second, i.e.

$$N(\psi,\lambda,E) = 0.2 \times 10^{-3} \times 53 \sum_{t=t_{inj}}^{11\,ms} n(\psi,\lambda,E,t) \qquad (3.8)$$

where $n(\psi,\lambda,E,t)$ = spectrum at time t.

3.4 Output

Because the volume of output is so large it was written in a catalogued file on magnetic disc. The file contains the matrices $N_{//}(\psi,\lambda,E)$ and $N_{Total}(\psi,\lambda,E)$, both of which are 60 × 61 × 5 dimensionally. These two matrices then provided the source data for analysis by several other programs each of which was interested in some particular aspect only. The results of most of this analysis have been published in references (1) and (3).

4. LIMITATIONS OF THE PROGRAM

The series approximations give rise to some errors in the calculations. The values computed largely agree with those published[7,8], but in the region of overlap of the two approximations the errors are $\leqslant$ 1% whereas elsewhere the errors are < 0.1%. The resulting errors in the calculated spectrum are at worst of the order of a few percent. These errors are only observable on the rapidly rising edges when the spectrum intensity is several orders of magnitude down from the peak. On these edges the figures are the result of sums involving a few terms from the large argument approximation only and consequently the error is at its worst.

A second source of error is the treatment of the energy variation during the acceleration cycle. The zero order trapezoidal integration (eqn.(3.8)) gives rise to errors $\sim$ 1% in the integrated spectrum.

The effect of errors generated by the program is considerably smaller than that caused by variations in the synchrotron which give rise to variations in intensity, orbit radius and beam size. For this reason no great effort was devoted to refining the algorithms any further.

5. RESULTS AND CONCLUSIONS

The results of these calculations have been presented elsewhere, the calculation of the total spectrum being the first step in calculating spectra for specific instruments and beam lines.

The program has generated data which have been used to produce source tables for many general and specific conditions in the NINA synchrotron and the SRS storage ring.

A listing of the computer program is available from the author.

REFERENCES

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5. R.A. Mack, CEA Report No. CEAL-1027.

6. J. Lang, SRC Astrophysics Research Unit Report, ARU(1), (1969).

7. G.N. Watson, A Treatise on the Theory of Bessel Functions, (London: Cambridge University Press, 1966).

8. H.W. Ellis and J.R. Stevenson, Computer calculations and numerical tabulations of some MacDonald functions. Georgia Institute of Technology Report, AFOSR 70-1892, (1970).

FIGURE CAPTIONS

Fig.1 Flow chart for the whole program.

Fig.2 Subroutine for the evaluation of the Bessel Functions with argument ≤ 3.5.

Fig.3 Subroutine for the evaluation of the Bessel Functions with argument > 3.5.

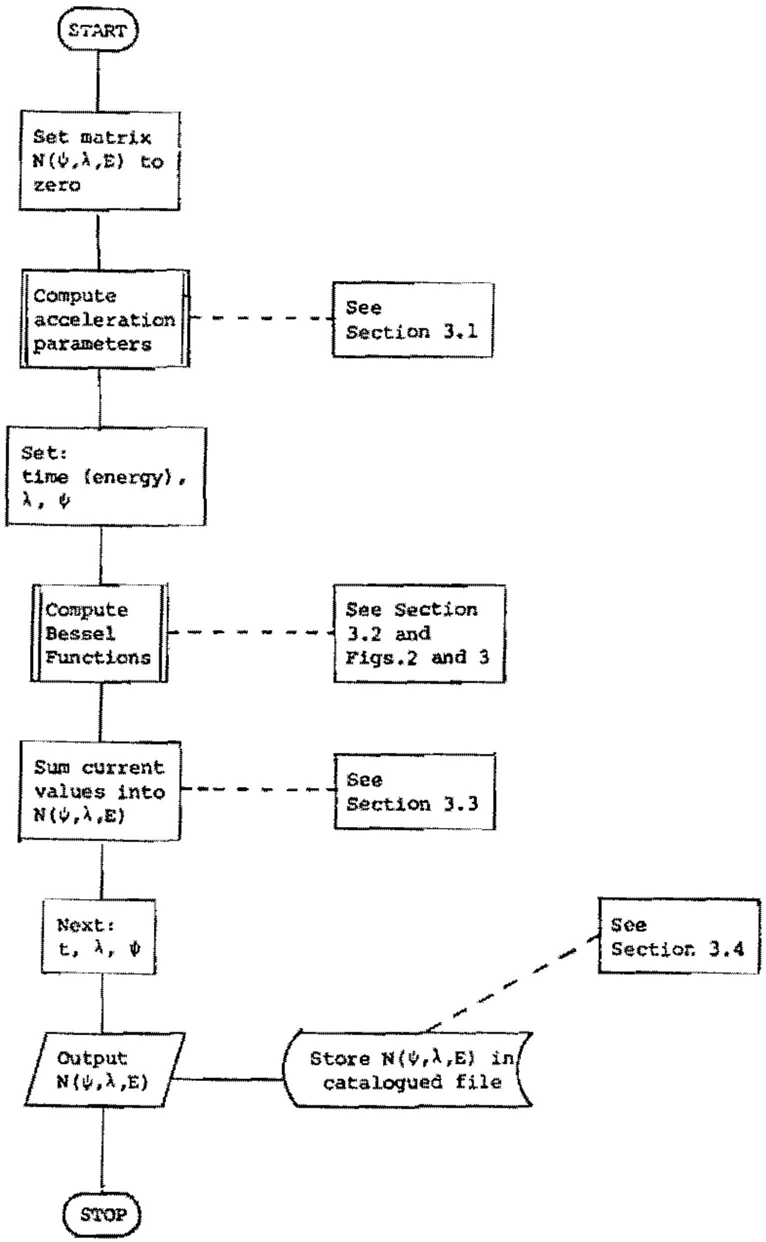

Fig. 1

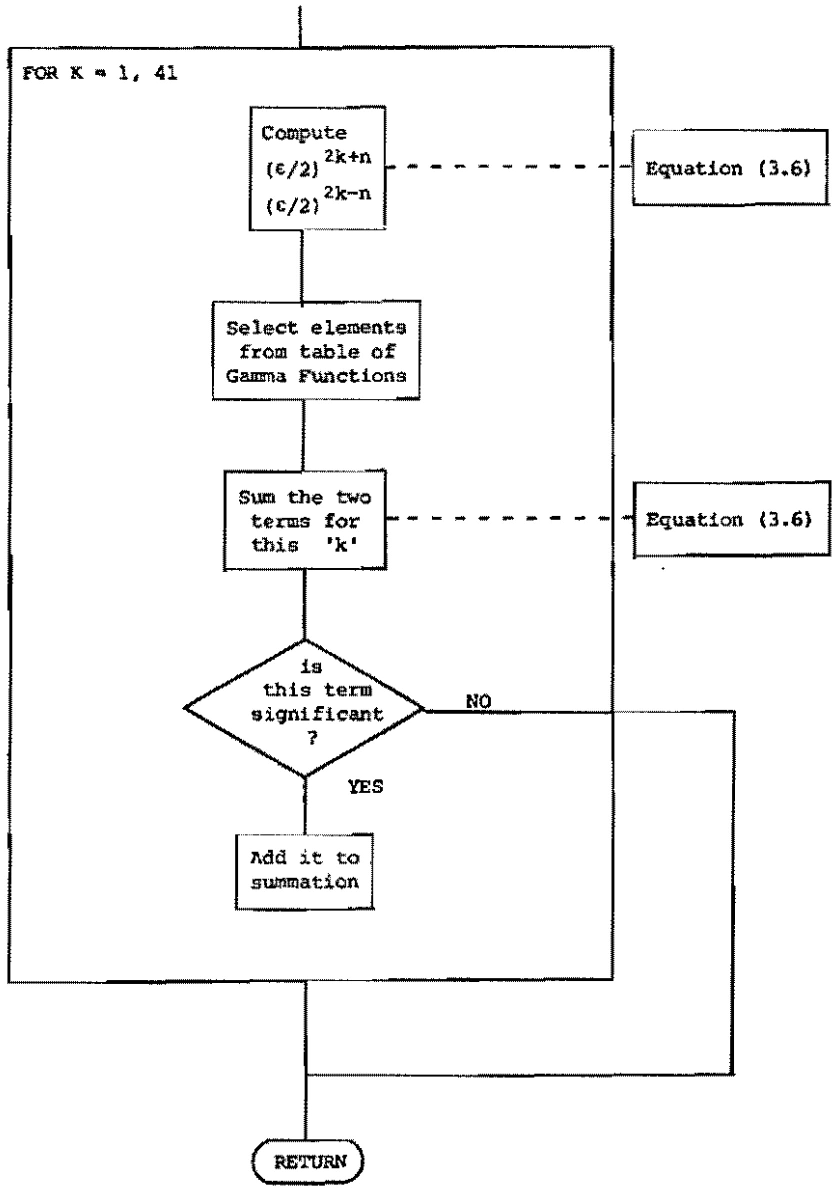
FOR K = 1, 41
Compute
(ε/2) 2k+n
(ε/2) 2k-n
Equation (3.6)
Select elements from table of Gamma Functions
Sum the two terms for this 'k'
Equation (3.6)
is this term significant ?
NO
YES
Add it to summation
RETURN

Fig. 2

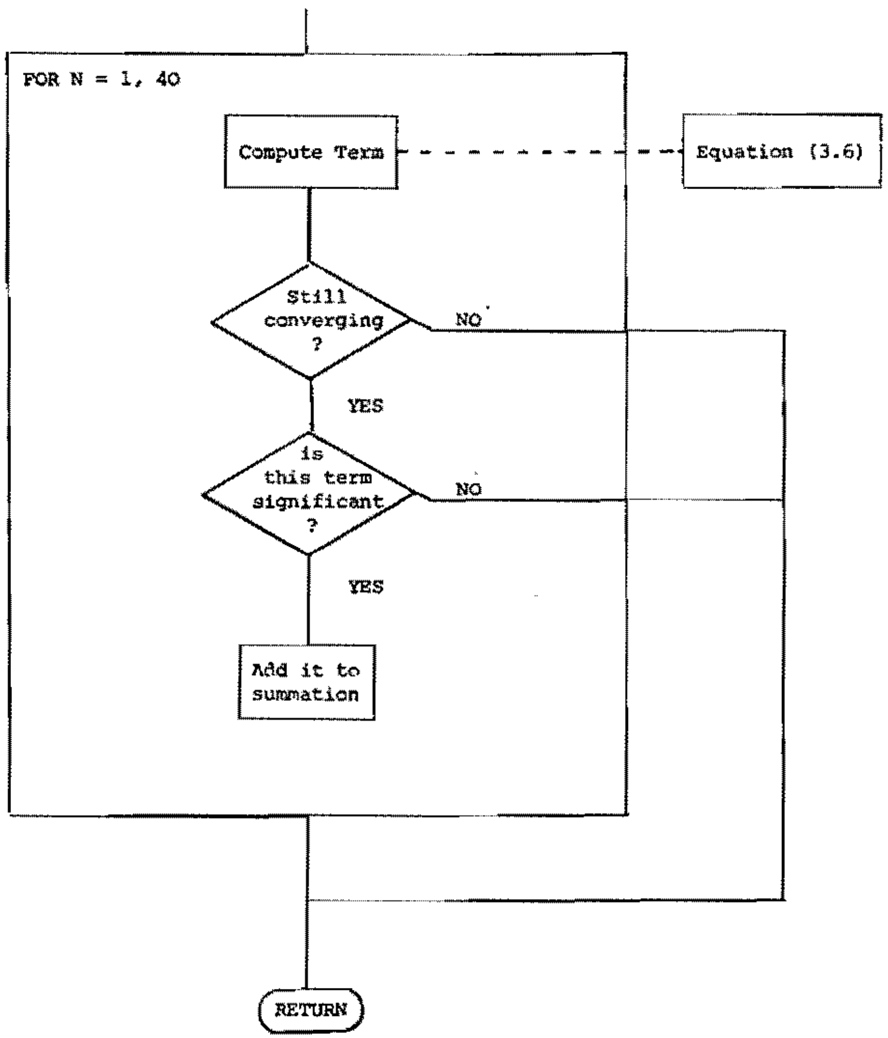
FOR N = 1, 40
Compute Term
Equation (3.6)
Still converging ?
NO
YES
is this term significant ?
NO
YES
Add it to summation
RETURN

Fig. 3