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CALCULATION OF SPECTRUM AND ANGULAR DISTRIBUTION NEAR THE PEAK OF AN UNDULATOR

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An undulator produces a complicated spectrum with peaks and a strong variation of spectrum with angle. However, in order to exploit its high spectral brilliance, the undulator will be used mainly selecting a narrow angle around $\theta = 0$ ($\theta \ll 1$) and with the monochromator tuned near the peak ($\Delta\lambda/\lambda \ll 1$ ($\sim$1-2%)). Therefore it is of interest to study simple approximations which could be valid in most practical cases.

While various kinds of computer programs written for general synchrotron radiation and undulator radiation are complicated and take a long computer time, near-peak approximations are simple and can be run on personal computers.

We consider here the (most common) case of a plane sinusoidal undulator. The formulas use here are a straightforward approximation of the formulas derived by Bessonov and coworkers, that are reminded in Fig. 1. The approximate formulas are summarised in in Fig. 2. These are utilised in two programs, of which we enclose the list and a few examples of results. These programs are written in "basic" for the Tektronix 4052, a rather primitive form of "basic", which should need almost no changes for other computers, except for graphic commands. They run in a few minutes (could run in a fraction of a minute with a compiler).

1.- FLUX AND LINESHAPE

This program plots spectral flux as a function of relative detuning $\Delta\lambda/\lambda$. The flux is in units relative to the ideal peak flux (which can be calculated by the program in ESRP/IRM- /84). The ideal flux (which is =0 for $\Delta\lambda/\lambda < 0$) is also shown as a dotted line.

Then it plots, in arbitrary units, the spectral brightness on axis, as a function of $\Delta\lambda/\lambda$, taking the electron angular spreads into account (in other words, this is the line shape through a pinhole on axis, of width $\propto (\lambda/L)^{\frac{1}{2}}$). The number of periods is indicated to get the scale for $\Delta\lambda/\lambda$.

The width of the plotted spectrum is 4/(I1*N1), where I1 = harm. number, and N1 = number of periods. To enter the desired values, edit from line 20 to 90.

2.- ANGULAR DISTRIBUTION FOR GIVEN DETUNING AND ELECTRON ANGULAR SPREADS

This program plots the diffraction pattern (single-electron rad. distribution) and the electron beam (horiz.) ang. spread, and the horizontal section of their convolution, i.e. the actual angular distribution of power per unit bandwidth, that is spectral brightness.

The spectral brightness is in arbitrary units, and the angular units in the x axis is 10 μrad.

A vertical section can be plotted by just interchanging the data for horiz. and vert. angular spread. To enter the desired values, edit from line 10 to 18.

TABLE I - Summary of general formulas for plane sinusoidal undulators

Spectral brightness:

Number of photons per unit time (i-th harmonic) and solid angle and relative bandwidth

N = num. of periods

$\alpha \simeq \frac{1}{137}$

$K = \frac{eB_0\lambda_0}{2\pi mc}$

$$\frac{dn/dt}{d\Omega\, d\omega/\omega} = \frac{1}{\hbar}\frac{dW}{d\Omega\, d\omega} = 4\alpha\gamma^2 \frac{I}{e} N^2 \xi f_i(\theta,\varphi)\, h^2(iN\Delta)$$

h: Fourier Transf. of B(z): for uniform amplitude:

$$h^2(iN\Delta) = \mathrm{sinc}^2(iN\Delta) = \left(\frac{\sin^2(\pi iN\Delta)}{\pi iN\Delta}\right)^2$$

$$f_i = f_{i_\parallel} + f_{i_\perp}$$

$$f_{i_\parallel} = \frac{1}{\xi}\left(\frac{iS_1+2S_2}{2\gamma\theta\cos\varphi} - \xi\gamma\theta S_1\cos\varphi\right)^2$$

$$f_{i_\perp} = \xi\gamma^2\theta^2 S_1^2 \sin^2\varphi$$

$$S_1 = \sum_{p=-\infty}^{+\infty} J_{i+2p}(z)J_p(y) \qquad S_2 = \sum_{p=-\infty}^{+\infty} pJ_{i+2p}(z)J_p(y)$$

$$\xi = \frac{i}{(1+\frac{K^2}{2})(1+\frac{\gamma^2\theta^2}{1+\frac{K^2}{2}})} \qquad \omega_i = 2\gamma^2\omega_0\xi \qquad \omega_0 = 2\pi c/\lambda_0$$

$$-\Delta = \frac{\omega-\omega_i}{\omega_i}$$

$$z = 2\gamma\theta K\xi\cos\varphi \qquad y = \frac{iK^2/4}{1+K^2/2}$$

Spectral flux:

$$\frac{dn/dt}{d\omega/\omega} = \frac{dn/dt}{d\lambda/\lambda} = \frac{1}{\hbar}\frac{dW}{d\omega} = 2\alpha\frac{I}{e} N F_i(\Delta) * \mathrm{sinc}^2(iN\Delta)$$

$$F_i(\Delta) = F_{i_\parallel} + F_{i_\perp} \qquad F_i = \int_0^{2\pi} f_i\, d\varphi$$

= convolution: $f(x) * g(x) = \int f(x')g(x-x')dx'$

TABLE II - Approximations for $\gamma\theta \ll 1$, $\Delta\lambda/\lambda \ll 1$

Let $\Delta\lambda/\lambda$ = detuning from the peak at $\theta=0$

$$\Delta = \frac{\Delta\lambda}{\lambda} - \frac{\gamma^2\theta^2}{1+\frac{K^2}{2}} = \frac{\Delta\lambda}{\lambda} - x^2 \qquad \left(\text{let } x^2 = \frac{\gamma^2\theta^2}{1+\frac{K^2}{2}}\right)$$

$\text{sinc}^2 iN\Delta$ is the diffraction pattern (single electron rad. pattern), with circular symmetry. Convoluted with ang. spreads, gives actual radiation ang. distribution

$f_i(\theta,\varphi)$:

odd harmonics:

$$f_{i_{\parallel}} = yQ_1^2\left[1-x^2-4ix^2\left(\frac{Q_2+yQ_3}{Q_1}\right)\cos^2\varphi\right] \qquad f_{i_{\perp}} = 4i^2yx^4Q_2^2\sin^2\varphi\cos^2\varphi$$

even harmonics:

$$f_{i_{\perp}} = ix^2J_{i/2}^2(y)\sin^2\varphi \qquad f_{i_{\parallel}} = \frac{i^2}{1+\frac{K^2}{2}}x^2\left[yQ_1+J_{i/2}(y)\right]^2\cos^2\varphi$$

let: $Q_1 = \frac{J_{i-1}}{2}(y) - \frac{J_{i+1}}{2}(y)$, $\quad Q_2 = \frac{J_{i-1}}{2}(y) + \frac{J_{i+1}}{2}(y)$,

$$Q_3 = Q_1 + \frac{J_{i-3}}{2}(y) - \frac{J_{i+3}}{2}(y).$$

Spectral brilliance at $\theta=0$ (lineshape through pinhole) with angular spread:

The angular distribution of electrons:

$$G(\theta,\varphi) = \frac{1}{2\pi\sigma_x'\sigma_y'}\exp\left[-\frac{\theta^2\cos^2\varphi}{2\sigma_x'^2} - \frac{\theta^2\sin^2\varphi}{2\sigma_y'^2}\right] = e^{-p\left[1-(1-\beta)\cos^2\varphi\right]} =$$

$$= e^{-\frac{p}{2}(1+\beta)}\, e^{+\frac{p}{2}(1-\beta)\cos 2\varphi}; \qquad \text{where } p = \frac{\theta^2}{2\sigma_{x'}^2}, \quad \beta = \frac{\sigma_{y'}^2}{\sigma_{x'}^2}$$

$$\bar{f}_i\left(\frac{\Delta\lambda}{\lambda}\right) = \bar{f}_i^{(\infty)}\left(\frac{\Delta\lambda}{\lambda}\right) * \text{sinc}^2 iN\frac{\Delta\lambda}{\lambda}$$

$$\bar{f}_i^{(\infty)}\left(\frac{\Delta\lambda}{\lambda}\right) = \iint f_i(\theta,\varphi)G(\theta,\varphi)\delta\left(\frac{\Delta\lambda}{\lambda} - x^2\right)d\varphi\,\theta d\theta =$$

$$= \frac{yQ_1^2}{\sigma_x'\sigma_y'}e^{-\frac{p}{2}(1+\beta)}\left\{\left(1-A\frac{\Delta\lambda}{\lambda}\right)I_0\left[\frac{p}{2}(1-\beta)\right] - (A-1)\frac{\Delta\lambda}{\lambda}I_1\left[\frac{p}{2}(1-\beta)\right]\right\}$$

where:

$A = 1+2i(Q_2+yQ_3)/Q_1$; $\quad \int_0^{2\pi} e^{a\cos x}\cos mx\,dx = 2\pi I_m(a)$ modified Bessel function.

```
1 REM undul. near peak flux & lineshape
10 INIT
20 P=32    number of the peripheral device: screen or plotter
30 N1=100  number of periods
40 I1=1    harmonic number
50 K=1     deflection parameter
60 N=8     this determines resolution (and execution time) (for ex. N=4 for fast calculation,
70 S1=1.6E-5   horizontal angular spread of electron beam     N=12 for better resolution)
80 S2=1.2E-5   vertical angular spread
90 G=10000     γ (electron energy)
100 N=N*I1
110 U=1/(N1*N)   in this case the Bessel functions are the ordinary ones, Jm(Y1)
120 Y1=I1*K*K/(1+K*K/2)^4   goes to the subroutine necessary for the calculation
130 U1=-1                                                    of A in line 180
140 GOSUB 590
150 WINDOW -4*N/I1,4*N/I1,0,1/N1
160 AXIS @P:N,1/N1*0.1,0,0
170 MOVE @P:-4*N/I1,0
180 A=1+2*I1*(Q2+Y1*Q3)/Q1
190 B1=S2*S2/S1/S1
200 Y2=U*(1+K*K/2)^(4)*S2*S2*G*G)
210 FOR Y=-4*N/I1 TO 4*N/I1      beginning of convolution
220 S=0.01/N1/I1/I1*(1-U1)^2     usually ≃ 0 (rough adjustment)
230 FOR I=-4*N/I1 TO Y
240 D=PI*I/N*I1
250 IF D=0 THEN 290
260 C=SIN(D)/D   homogeneous lineshape due to finite number of periods (spectrum at
270 GO TO 290                                                given θ for S1=S2=C)
280 C=1
290 IF U1=-1 THEN 400   to calculate flux; the second time, after returning from 540,
300 U1=0                                  it goes on to 300 to calculate lineshape
310 Y1=Y2*(Y-I)*(1-B1)
320 GOSUB 800    to calculate I0(Y1)
330 W0=Z
340 U1=1
350 GOSUB 800   to calculate I1(Y1)
360 W1=Z
370 B=((1-A*U*(Y-I))*W0-(A-1)*U*(Y-I)*W1)*EXP(Y2*(I-Y)*(1+B1))  ideal line
380 B=B/I1*N/8  in order to avoid to go out of scale              shape on pinhole at θ=0
390 GO TO 420                (the scale is arbitrary)             (N1→∞ with given S1, S2)
400 B=1-A*U*(Y-I)   ideal (N1→∞) integrated spectrum (flux
410 IF I=Y THEN 440                as a function of Δλ/λ)
420 S=S+C*C*U*B   ⟶ S(Y) = ∫C²(I)B(I-Y)dI
430 NEXT I
440 S=S+C*C*U*0.5   we take the average value at the discontinuity
450 DRAW @P:Y,S*I1  plots the result of convolution: first time flux, second time lineshape
460 NEXT Y
470 MOVE @P:0,1
480 IF U1=1 THEN 550   if lineshape has already been calculated, it stops (line 580)
490 FOR I=0 TO 4*N/I1                  }
500 MOVE @P:I,(1-A*U*I)^N1             } prints as a dotted line the ideal spectrum B(I)
510 DRAW @P:I,(1-A*U*I)*1/N1           }
520 NEXT I
530 U1=1    in order to calculate modified Bessel function Im(Y1)
540 GO TO 170   in order to calculate lineshape
550 HOME @P:
560 PRINT @P:I1;"-TH HARM., NUM.PER.= ";N1
570 PRINT @P:"ANG.SPR.: ";S1;" , ";S2
580 STOP    end of program
```

```
590 REM calc. of coeff. "A"
600 U1=(I1-1)/2
610 U2=1
620 GOSUB 800
630 Z1=Z
640 U1=(I1+1)/2
650 GOSUB 800
660 Z2=Z
670 U1=(I1-3)/2
680 U2=SGN(U1)
690 U1=ABS(U1)
700 GOSUB 800
710 Z3=Z
720 U1=(I1+3)/2
730 U2=1
740 GOSUB 800
750 Z4=Z
760 Q1=Z1-Z2
770 Q2=Z1+Z2
780 Q3=Q1+Z3-Z4
790 RETURN                                  end of subroutine for calculation of A
800 REM BESSEL: ORDER U1,ARG.Y1(v1=-1 ord.,v1=1 modif.)
810 IF U1=1 AND Y1>4 THEN 1060                  ↳J          ↳I
820 Z=0
830 F1=1
840 FOR I2=1 TO U1
850 F1=F1*I2
860 NEXT I2
870 H=0
880 K2=1
890 GO TO 920
900 K2=K2+H
910 F1=F1*(U1+H)
920 IF Y1=0 THEN 950
930 F0=(U1*Y1*Y1/4)↑H/K2
940 GO TO 960
950 F0=1
960 Z=Z+F0/F1*U2
970 IF Y1=0 THEN 1000
980 IF ABS(F0/F1)*(Y1/2)↑U1<1.0E-3 THEN 1030
990 GO TO 1010
1000 IF ABS(F0/F1)<1.0E-4 THEN 1030
1010 H=H+1
1020 GO TO 900
1030 IF Y1=0 AND U1=0 THEN 1050
1040 Z=Z*(Y1/2)↑U1
1050 RETURN
1060 REM MODIF BESSEL FOR LARGE ARGUMENT
1070 Z0=1
1080 I3=1
1090 H=1
1100 H=H*(2*I3-1)*(2*I3-1)/(8*I3*Y1)
1110 Z0=Z0+H
1120 IF H<1.0E-3 THEN 1150
1130 I3=I3+1
1140 GO TO 1100
1150 Z0=Z0/SQR(2*PI*Y1)
1160 Z=Z0
1170 RETURN
```

```
F
1  REM  ANGULAR DISTRIBUTION (D,S1,S2)
2  INIT
4  P=32    number of the peripheral device (screen or plotter)
6  W=3     width (number of standard deviations in the case of the gaussian)
8  Q=8     determines number of points and then resolution
9  U0=1.0E-5     spacing of ticks in horizontal axis
10 S1=1.6E-5     electron beam horizontal angular spread
11 S2=1.2E-5     electron beam vertical angular spread
12 L1=4.0E-9     output wavelength λ
14 D=0.017       detuning Δλ/λ
15 G=10000       gamma (electron energy)
16 K=2.5         deflection parameter of undulator
17 I1=1          harmonic number
18 L9=5          total length of undulator
19 L9=5
23 X0=G*G/(1+0.5*K*K)
24 L0=2*L1*X0    undulator period
25 N0=L9/L0      number of periods
26 PRINT"NUM.PER.:";INT(10*N0)/10;"  PER.:";INT(100*L0);" CM."
28 PRINT"WAVELENGTH: ";INT(L1*1.0E+11)/10;" ANGS."
30 T8=SQR(L1/L9)
31 T0=SQR(D/X0)
32 IF D<0.5*L0/L9 THEN 60
36 T9=1/(2*L9/L0*G*SQR(D))
55 T1=T9
57 GO TO 65
60 T1=T8
62 T0=T8
65 IF S1>T1 THEN 75
70 U=T1/Q
72 GO TO 100
75 U=S1/Q
100 N=INT(W*S1/U)
110 M=INT(W*S2/U)
120 L=INT(W*T0/U)
130 PRINT "RESOL.=";INT(10000000*U)/10;" MICRORAD"
132 PRINT "DETUNING: ";D*N0
140 DIM A(2*N+1,2*M+1)
150 DIM B(2*L+1,2*L+1)
160 FOR I2=-N TO N
170 FOR J2=-M TO M
180 H=U*U*(I2*I2/S1/S1+J2*J2/S2/S2)/2
190 I=I2+N+1
200 J=J2+M+1
210 A(I,J)=EXP(-H)
220 NEXT J2
230 NEXT I2
```

this is to determine number of points, and then dimension of arrays A,B,C not too big (mem. overflow) and not too small (low resolution) can be adjusted by varying Q (line 8)

calculates gaussian

```
240 FOR I2=-L TO L
250 FOR J2=-L TO L
260 U=PI*I1*L9/L0*(X0*U*U*(I2*I2+J2*J2)-D)
270 I=I2+L+1
280 J=J2+L+1
290 IF U=0 THEN 320
300 B(I,J)=SIN(U)/U*(SIN(U)/U)
310 GO TO 330
320 B(I,J)=1
330 NEXT J2
340 NEXT I2
```

calculates diffraction pattern (single electron distribution)

```
350 WINDOW -L-N,L+N,0,1
360 AXIS @P:U0/U,0.1
370 MOVE @P:-N,A(1,M+1)
380 FOR I=2 TO 2*N+1
390 DRAW @P:I-N-1,A(I,M+1)
400 NEXT I
410 MOVE @P:-L,B(1,L+1)
420 FOR I=2 TO 2*L+1
430 DRAW @P:I-L-1,B(I,L+1)
440 NEXT I
450 MOVE @P:0,1
```

plots horizontal section of gaussian

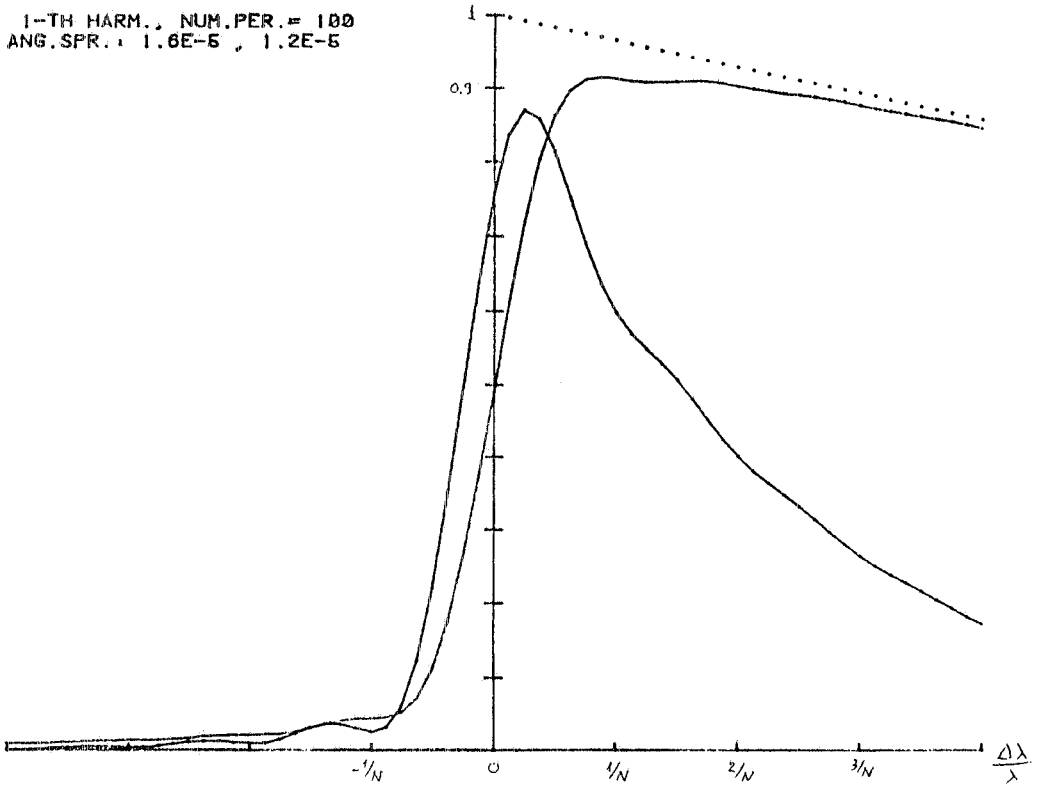
plots section at diffraction pattern

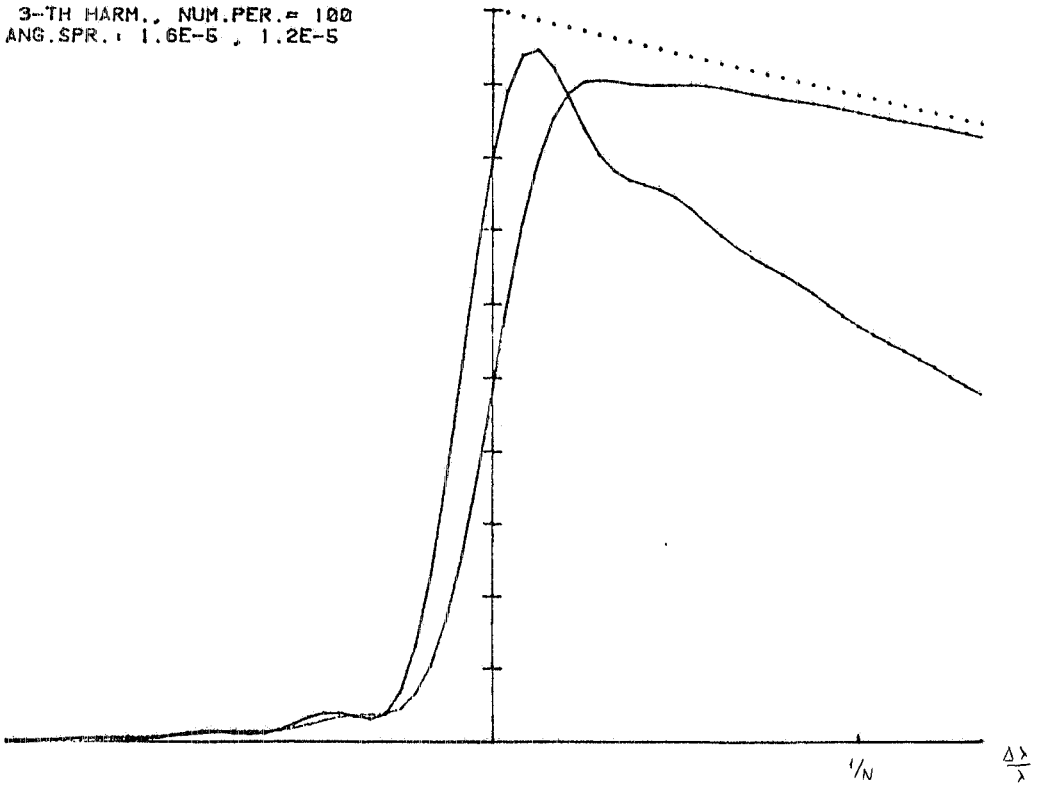
```
460 DIM C(L+N+1)
470 N9=L*L*M*N/W↑4
480 FOR Y=0 TO L+N
490 C(Y+1)=0
500 FOR I3=-N TO N
510 IF I3<Y-L OR I3>Y+L THEN 660
520 I0=I3+L+1
530 I=I3+N+1
540 FOR J3=-N TO M
550 IF J3>L OR J3<-L THEN 650
560 J=J3+M+1
570 J0=J3+L+1
580 C(Y+1)=C(Y+1)+A(I,J)*B(I0-Y,J0)
590 IF Y<2 THEN 640
600 IF C(Y+1)<C(Y) AND C(Y)>C(Y-1) THEN 620
610 GO TO 650
620 M1=C(Y)
630 GO TO 650
640 M1=C(1)
650 NEXT J3
660 NEXT I3
670 NEXT Y
```

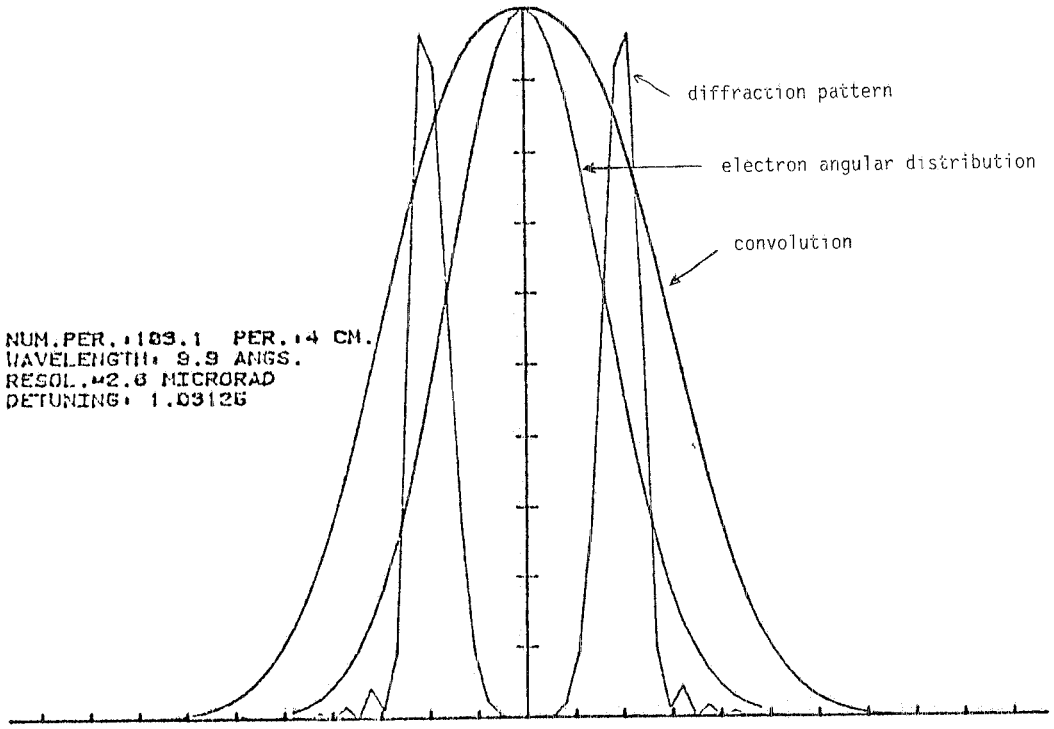
convolution A ⊛ B (horizontal section)

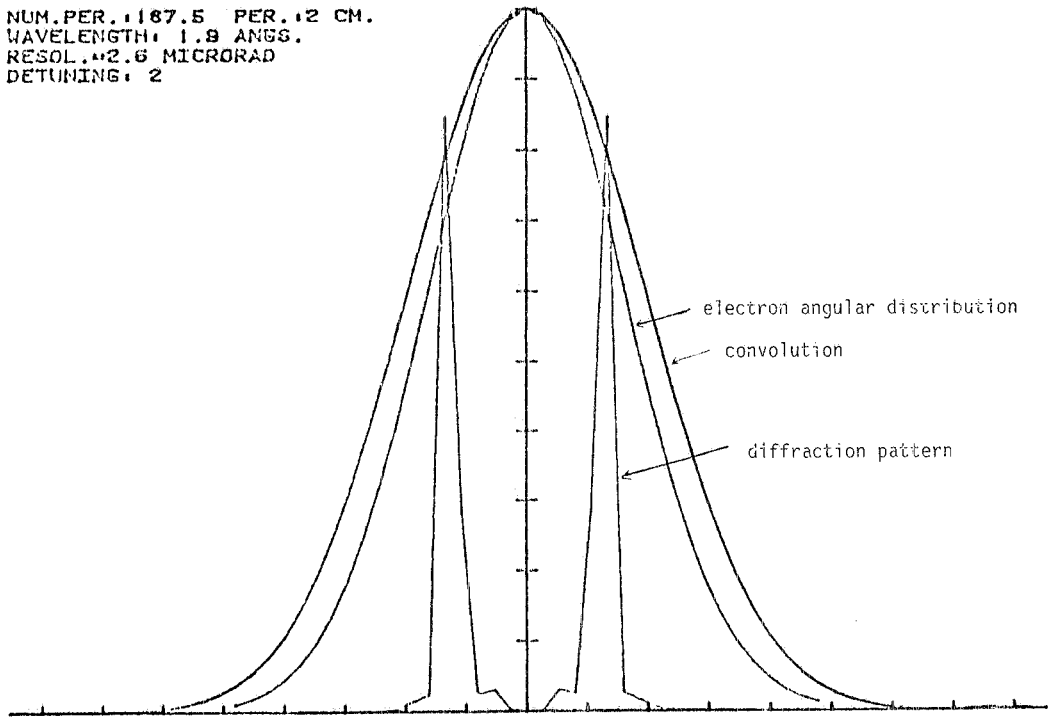
```
680 FOR Y=0 TO L+N
690 DRAW @P:Y,C(Y+1)/M1
700 NEXT Y
710 MOVE @P:0,0
720 FOR Y=0 TO L+N
730 DRAW @P:-Y,C(Y+1)/M1
740 NEXT Y
```

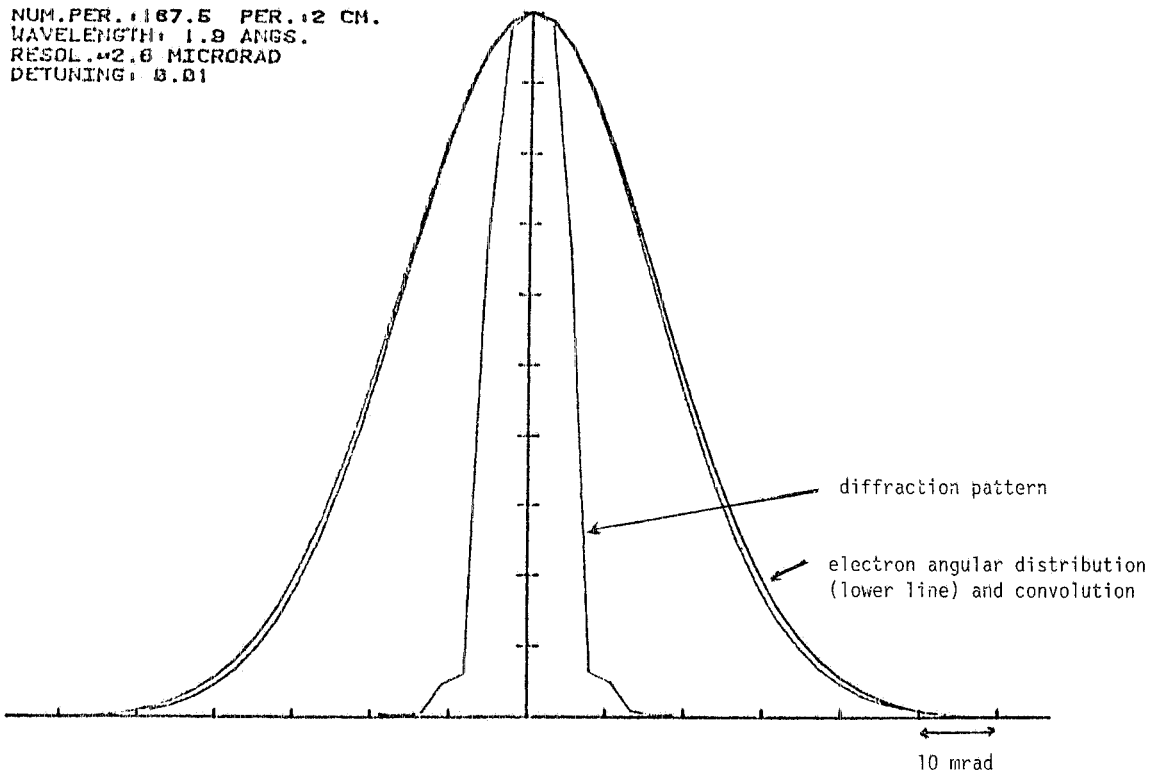
draws convolution


1-TH HARM., NUM.PER.= 100
ANG.SPR.: 1.6E-5 , 1.2E-5
1
0.9
-1/N
0
1/N
2/N
3/N
Δλ/λ


3-TH HARM., NUM.PER.= 100
ANG.SPR.: 1.6E-5 , 1.2E-5
1/N
Δλ/λ


diffraction pattern
electron angular distribution
convolution
NUM.PER.=183.1 PER.=4 CM.
WAVELENGTH= 9.9 ANGS.
RESOL.=2.6 MICRORAD
DETUNING= 1.03125


NUM.PER.=187.5 PER.=2 CM.
WAVELENGTH= 1.9 ANGS.
RESOL.=2.6 MICRORAD
DETUNING= 2
electron angular distribution
convolution
diffraction pattern


NUM.PER.=167.5 PER.=2 CM.
WAVELENGTH= 1.9 ANGS.
RESOL.=2.6 MICRORAD
DETUNING= 0.01
diffraction pattern
electron angular distribution
(lower line) and convolution
10 mrad