

W.Quapp and J.M.Bofill

Sliding Paths for Series of Frenkel – Kontorova Models–  
A contribution to the concept of 1D – superlubricity

Supplementary Material 3

MF 1/2 N = 6 ... × 20 with runaways 30, 35, 40

```
### ## ## ## ## ## ## ## ## == HALF ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
  quapp@uni - leipzig.de phone x (0) 341 × 97 × 32 137
### ## ## ## ## ## ## ## ## == HALF ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

N = 6 global minimum for Misfit 1/2

k = 1.0

as = 6.283185307180

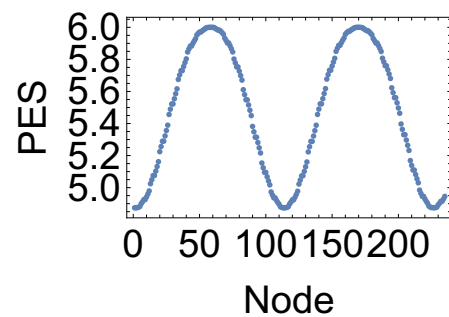
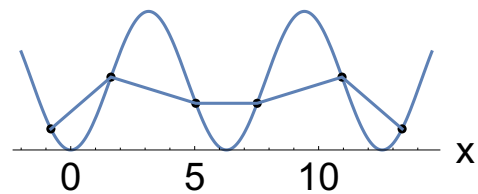
a0 = 0.5 \* as

ENERGY 4.874185069334626

SetX = {-0.80100645953, 1.6225292843,  
5.0447272235, 7.5216431268, 10.94384104976, 13.3673768724}

Eigenvalues

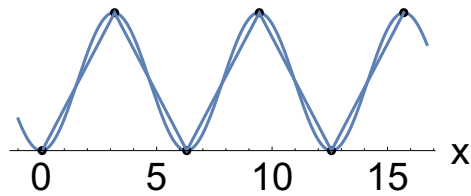
{3.96215, 3.16948, 2.37378, 1.51845, 0.634603, 0.282599}



```

SP energy = 5.99887 and by 171
node60 = { 0.0416497213, 3.1790433158, 6.3054496831,
9.4479999482, 12.5726880244, 15.7056327967}
next ' iMin ' by 113 energy = 4.876459
node113 = {0.7499989468, 4.6173638262, 7.4892401984,
11.2953325950, 14.1460171044, 17.9966624531}
next ' gMin ' by 228 energy = 4.87798
node228 = {5.4817093928, 7.9053216147, 11.3276162292,
13.8045321490, 17.2266333435, 19.6500928034}

```



```

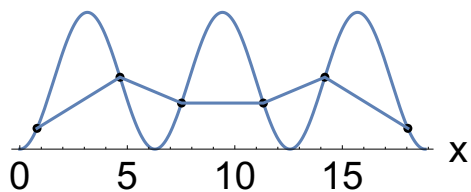
node113 = {0.7499989468, 4.6173638262, 7.4892401984,
11.2953325950, 14.1460171044, 17.9966624531}
Setxx = node113

SetX /. {A[1] → 0.051007393493551115, A[2] → 0.04329202390946741,
A[3] → 0.03240302838670783, A[4] → 0.032580004714758665,
A[5] → 0.04288286951171692, A[6] → 0.05188704327013859}

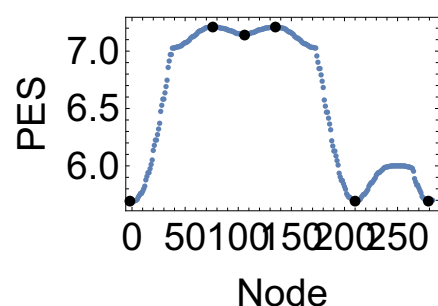
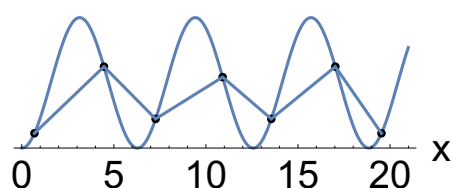
```

glob Min

```
{0.801006, 4.66066, 7.52164, 11.3279, 14.1889, 18.0485}
```



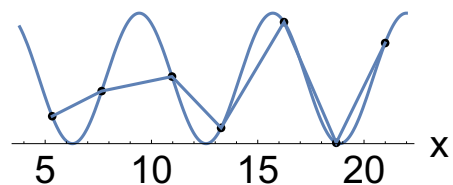
```
### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
N = 7 minimum HALF
ENERGY 5.6929210557125
SetX = {0.6862018214003, 4.461397762968, 7.267926930656,
        10.907585296022, 13.551112210789, 17.0277682813, 19.53575770545}
Eigenvalues
{4.03685778236836, 3.4550552007065405, 2.6039411473177836, 2.1344578905957374,
 1.1225921158775711, 0.4888591668855031, 0.2271057131865678`}
```



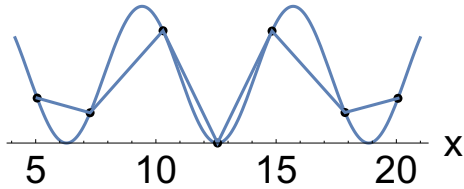
```

Half N = 7 SP very high
node80 = {3.1415926534, 6.2829378224, 9.4240355066,
12.5658756449, 15.7072208138, 18.8493084368,
21.9911485749}
ENERGY 07 is energy = 7.9999999999999
usual SP energy = 7.2105789
node160 = {5.3306657357, 7.6583917107, 10.9670508772,
13.2761168086, 16.2368240133, 18.6929811617,
20.9932025219}
iMin energy = 7.1438914
node190 = {5.0608113128, 7.2634648287, 10.2967713825,
12.564465107, 14.830253326, 17.865319291, 20.0675354477}
SetX = node160
ENERGY 07 is 6.156568

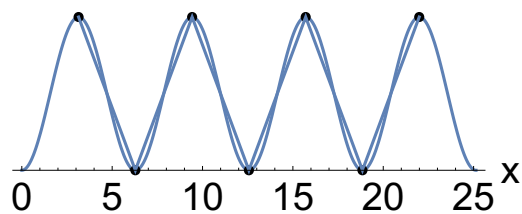
```



```
iMin energy = 7.1438914
node190 = {5.0608113128, 7.2634648287, 10.2967713825,
12.5644651074, 14.8302533266, 17.8653192915,
20.0675354477}
```

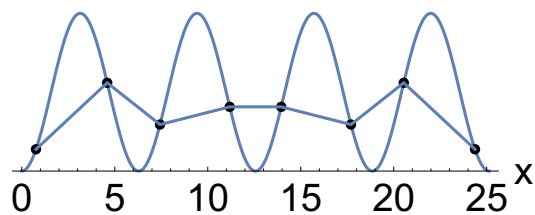


```
### ### ### ### ### # N = 7 global SP HALF ### ### ### ### ### #
SetX = {3.141592653590205,
6.283185307179793, 9.424777960769587, 12.566370614359176,
15.707963267948765, 18.849555921538556, 21.991148575128143}
Eigenvalues
{4.0728647391297, 3.6510934089372, 3.191842138507, 0.7261094450358,
-0.43966575070322, -0.37720285397296, 0.174958873066718}
```



Energy 8.0

```
N = 8 global minimum HALF new
### ### ### ### ### HALF ### ### ### ### ### ### ### ### ###
Energy 6.60798
SetX = {0.7613886429488335, 4.5929085969503625,
7.431557859970808, 11.182305154811159, 13.950436048937284,
17.701183260068426, 20.53983252785431, 24.37135251385667}
Eigenvalues
{4.084413743253319, 3.6328247629020103,
2.9322083976462254, 2.3570647592501004, 1.7246853361952073,
0.9495808036479993, 0.4589948110286991, 0.2608319623233443`}
```



it is N = 8 global minimum

```

SP node 26 energy = 7.902314
node26 = {0.5709731433, 4.2526902501, 7.0382211519,
10.5090668267, 13.0959413481, 16.1879787902,
18.8182232887, 21.4171402807 }
gMin ? node 7
node7 = {-0.2823755439, 3.1570571865, 6.5809819483,
10.2983628737, 13.2490998106, 16.8307842929,
19.5106296566, 22.8049743290}

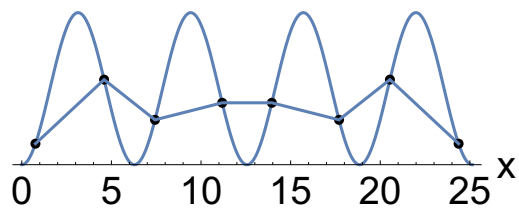
HALF N = 8 global minimum
Setxx = {-0.2823755439, 3.1570571865, 6.5809819483,
10.2983628737, 13.2490998106, 16.8307842929,
19.5106296566, 22.8049743290}

Energy 6.607975990986515

SetX = {0.7613886862708998, 4.5929086884036705,
7.431557937563794, 11.182305148736686, 13.95043600908645,
17.701183274680673, 20.53983256111681, 24.371352588905435}

Eigenvalues
{4.084413743850526, 3.6328247605117396,
2.932208416687675, 2.357064765673025, 1.7246853321414708,
0.9495808196550044, 0.4589948231486102, 0.26083196998851343}

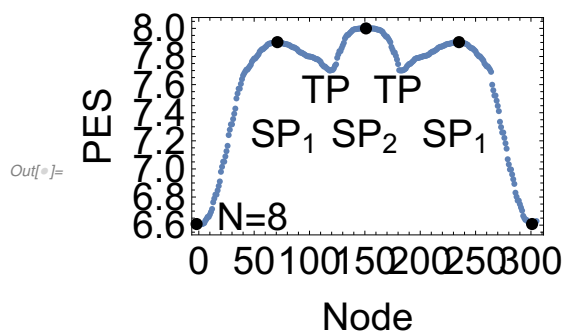
```



```

start
5.5218 × 7.97346 × 11.4180 × 13.9504
17.4655 × 19.9979 × 23.4425 × 25.8941
SP node71 energy = 7.9018666 detHess - 2.417
2.5719439390 × 6.2548232441 × 9.9093442884
13.0980406760 × 16.7937106402 × 19.6047284790
23.1011606452 × 25.7018887582
node186 energy = 7.907090 detHess - 3.393388
2.5617048074 × 6.2478253425 × 9.8985932810
13.0930766201 × 16.7902484814 × 19.6043877537
23.1036932131 × 25.7061713854
Min node253 energy = 6.62161 detHess 21.9513
5.5170139334 × 7.9696173916 × 11.4155424823
13.9483656642 × 17.4634187652 × 19.9954729781
23.4386156968 × 25.8893538274

```



```

SP node71 energy = 7.9022791
iSP2 ! node151 energy = 7.9999999 detHessian 0.99724
SP node235 energy = 7.902271
Min node302 energy = 6.607991

node70 = {3.6996016629, 6.3036795007, 8.9282500973,
12.0291962623, 14.6184320677, 18.0940778771,
20.8840869500, 24.5684842615}
node152 = {3.1307829454, 6.2723772816, 9.4031638026,
12.5555627989, 15.6971541902, 18.8495544487,
22.0019532345, 25.1435475711}

SetX = {3.1415926535904166, 6.283185307179793,
9.424777960769378, 12.566370614358963, 15.70796326794834,
18.849555921538343, 21.991148575127927, 25.132741228718135}

```

Eigenvalues

```

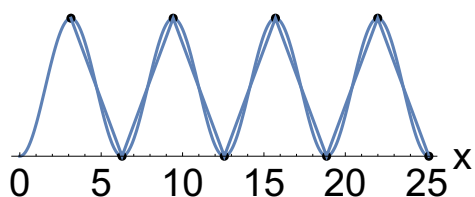
{{4.101002989615458, 3.732050807568878,
3.2592801267497657, 2.4142135623730936, 0.7407198732502391,
-0.41421356237309315, 0.26794919243112636, -0.10100298961545207},

```

```
node235 = {2.5851795721, 6.2637628699, 9.9229249516,
13.1042884854, 16.7980010375, 19.6050692080,
23.0977997687, 25.6963257486}
node301 = {5.5258433599, 7.9767224527, 11.4200783433,
13.9521911248, 17.4672446052, 20.0000088583,
23.4457219769, 25.8981813806}
```

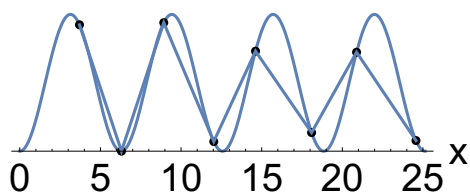
Energy 8.0

SetX = node152



sp2Half

```
node70 = {3.6996016629, 6.3036795007, 8.9282500973,
12.0291962623, 14.6184320677, 18.0940778771,
20.8840869500, 24.5684842615}
```



spHalfRiInnen

```
Inner distribution of atoms 3 : 2 : 2 : 1
Out      -- "  --      1 : 1 : 2 : 2 : 2
      Meanvalue is SP2 Right
```

Search below SP2 an iMin !

Setxx = node152

Energy 6.607975990987186

Hess

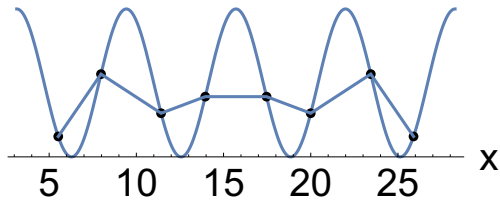
```
{{1.7238786291011732, -1., 0, 0, 0, 0, 0, 0},
{-1., 1.8808037497059131, -1., 0, 0, 0, 0, 0},
{0, -1., 2.409972305583472, -1., 0, 0, 0, 0},
{0, 0, -1., 2.185647617370332, -1., 0, 0, 0},
{0, 0, 0, -1., 2.185647617436202, -1., 0, 0},
{0, 0, 0, 0, -1., 2.4099723055224094, -1., 0},
{0, 0, 0, 0, 0, -1., 1.8808037498196648, -1.0},
{0, 0, 0, 0, 0, 0, -1., 1.72387862906145}}
```

```
SetX = {5.521796639331006, 7.973461955927407,
11.417997986120808, 13.950436045337973, 17.465490490626994,
19.997928549844072, 23.442464580085094, 25.894129896624502}
```

Eigenvalues

```
{4.084413744692757, 3.6328247584549054,
 2.9322084080284965, 2.3570647626572354, 1.7246853344708923,
 0.9495808146856901, 0.45899481460815816, 0.2608319660024745}
```

! iMin has same Energy like gMin ! is moved ok



iMINhalb

SP 186 energy = 7.9006625717

but node125 is Nothing ? TP only

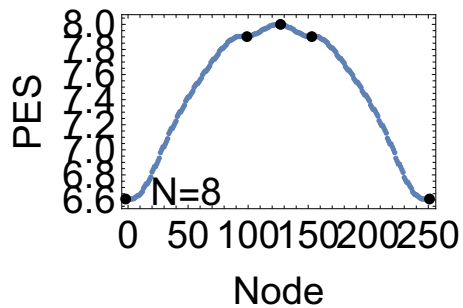
```
node02 = {5.5218 × 7.97346 × 11.418 × 13.9504 × 17.4655 ×
 19.9979 × 23.4425 × 25.8941}
```

```
node68 = {2.6424921443, 6.2992065140, 9.9844617193,
 13.1332242165, 16.8215046714, 19.6089051631,
 23.0857237599, 25.6758722547}
```

```
node186 = {2.4653556461, 6.1778719121, 9.7852692537,
 13.0399308127, 16.7506546802, 19.5975689021,
 23.1246856614, 25.7458272551}
```

```
node250 = {5.4695218256 × 7.9319491298 × 11.3913386783 ×
 13.9280252537 × 17.4429219989 × 19.9712609109 ×
 23.4004418323 × 25.8426358191}
```

wieder am Ausgangspunkt zurueck



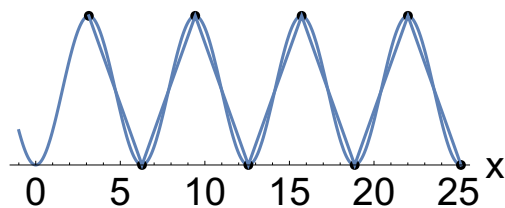
NT to EV1 of iMin goes over SP2 but without TPs



```

start
node02 = {5.5218000000 × 7.9734600000 ×
11.4180000000 × 13.9504000000 ×
17.4655000000 × 19.9979000000 ×
23.4425000000 × 25.8941000000}
  by node99 SP1 detHess - 2.5345 energy = 7.902361
and node127 detHess 0.989 energy 7.999961
  again SP2 NOTE : exists 2 x in different mirror form
Node 148 again SP1 ok
node98 = {3.6932627132, 6.3089989749, 8.9479913766,
12.0435179364, 14.6371039295, 18.1057158469,
20.8948167023, 24.5709004163}
node126 = {3.1397531274, 6.2841305437, 9.4308361218,
12.5727786392, 15.7225294855, 18.8591149771,
22.0065544420, 25.1399715749}

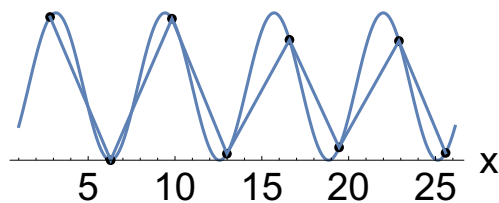
```



```

node 148 SP1
node148 = {2.8071435929, 6.2955594132, 9.8235241549,
12.9886742912, 16.5912047471, 19.4484525534,
22.8948804399, 25.5828422436}

```



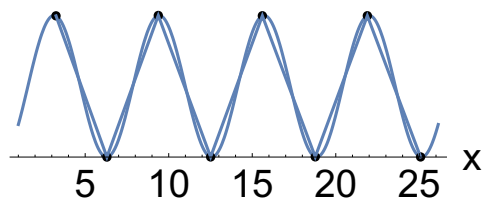
spHalfRiOut

```

node70 = {3.6996016629, 6.3036795007, 8.9282500973,
12.0291962623, 14.6184320677, 18.0940778771,
20.8840869500, 24.5684842615}
  von oben : ist SP ReInnen hier SP Re Out mix both
MIXXX = 0.5 * (node70 + node148)
{3.25337, 6.29962, 9.37589, 12.5089, 15.6048, 18.7713, 21.8895, 25.0757}

```

SetX = MIXXX

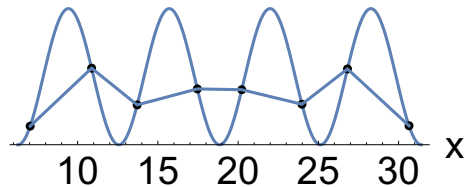


Global min by 248 detHess 20.20437

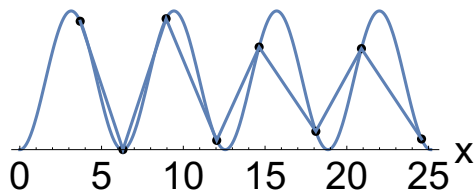
```
node247 = {0.7574856455, 4.5871921644, 7.4262136205,
11.1765225184, 13.9446647214, 17.6958423138,
20.5341388077, 24.3674566407} + 2. * Pi
```

```
SP node344 = { -0.5698827678, 2.0320107205, 5.5291743184,
8.3415426652, 12.0371434311, 15.2276321427,
18.8799665246, 22.5624642230}
```

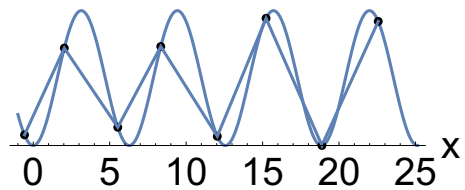
SetX = node247



SetX = node98

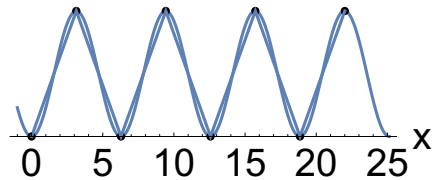


SetX = node344



```
SP2mirror = {0.0, 3.1397531274, 6.2841305437, 9.4308361218,
12.5727786392, 15.7225294855, 18.8591149771,
22.0065544420}
```

SetX = SP2mirror



Setxx = SP2mirror

```
{2.05412 × 10-13, 3.14159, 6.28319, 9.42478, 12.5664, 15.708, 18.8496, 21.9911}
```

Eigenvalues

```
{4.101, 3.73205, 3.25928, 2.41421, 0.74072, -0.414214, 0.267949, -0.101003}
```

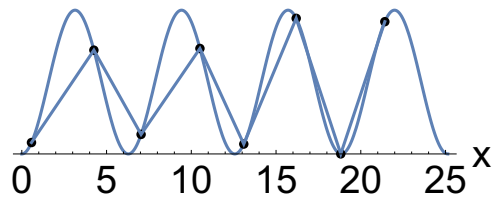
Setxx = SP2mirror + 0.456789

```
SetX = {0.5707106502647629, 4.252533660377795,
  7.038240189170832, 10.509275553542134, 13.096242439110503,
  16.188632211776692, 18.818649646930936, 21.41776565058075}
{0.570711, 4.25253, 7.03824, 10.5093, 13.0962, 16.1886, 18.8186, 21.4178}
```

### Eigenvalues

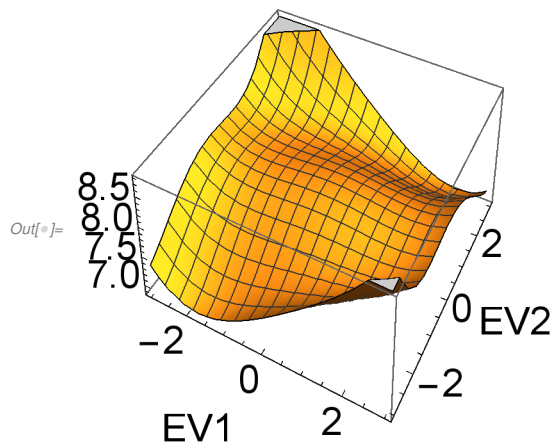
```
{4.10197, 3.71954, 3.22835, 2.36293, 1.03721, 0.463518, -0.281982, 0.162695}
```

old SP1 in ENERGY 7.902314855909



Search symm SP1 near SP2 ?

```
as = 6.283185307180
PlaX = 3.2533726279, 6.29961945695, 9.3758871261, 12.50893527675,
  15.6048184074, 18.771265215249997, 21.889483694950002, 25.07566325255} +
a * {0.8412609923560, 0.348461712529337, 0.3484617125293367,
  0.144337567297405, 0.144337567297404, 0.05978657793452398,
  0.059786577934523494, 0.02476441142835576} +
s * {-0.2748120509297, -0.02775683872625, 0.188738011057324,
  0.23555795315444436, 0.54172790590230, 0.360886090802114,
  0.5773809405856893, 0.2748120509297181}
note : a - EV ist non - sym, not a - sym !
a0 = 0.5 * as
plane[s_, a_] = Sum[1 - Cos[PlaX[[i]]], {i, 8}] +
  Sum[k/2. * (PlaX[[i + 1]] - PlaX[[i]] - a0)^2, {i, 7}]
```



search SP bei (2, 0) ...

```
iMinXX1 = {3.2533726279, 6.29961945695, 9.375887126, 12.5089352767,
  15.604818407, 18.771265215, 21.8894836949, 25.0756632525} -
  0.000111 * {0.8412609923560835, 0.34846171252933766,
    0.3484617125293, 0.144337567297405, 0.144337567297404,
    0.05978657793452, 0.059786577934523, 0.02476441142835} +
  2.000175 * {-0.27481205092971683, -0.027756838726255537,
    0.18873801105732, 0.23555795315444, 0.5417279059023,
    0.36088609080211, 0.5773809405856, 0.2748120509297}
{2.70361, 6.24406, 9.75336, 12.9801, 16.6884, 19.4931, 23.0443, 25.6253}
```

Setxx = iMinXX1

```
SetX = {2.5682093865062074, 6.252279370807958,
  9.905448338609204, 13.096243612936503, 16.792462646666532,
  19.604612123198347, 23.102091197374662, 25.703452836025882}
```

Eigensystem

```
{ {4.10197, 3.71954, 3.22835, 2.36292, 1.03721, 0.463518, -0.281982, 0.162696},
  { {-0.0957921, 0.377616, -0.320509, 0.580273, -0.398505,
    0.443616, -0.210905, 0.093302}, {0.180453, -0.642343,
    0.282043, -0.0927239, -0.20261, 0.53581, -0.328541, 0.17494},
  {-0.168824, 0.518022, 0.050288, -0.624383, 0.177909, 0.322703,
    -0.339297, 0.244656}, {-0.0454838, 0.100201, 0.109271, -0.236747,
    -0.227632, 0.425745, 0.38316, -0.734857}, {0.169415, -0.148624,
    -0.461061, 0.113534, 0.668336, 0.217585, -0.300395, -0.373482},
  {-0.333708, 0.10131, 0.590631, 0.28248, 0.0871379, -0.189319,
    -0.51589, -0.374377}, {0.828543, 0.366142, 0.372955, 0.154241,
    0.11211, 0.0491965, 0.0359823, 0.0169448}, {-0.318032, 0.000879714,
    0.320528, 0.30382, 0.49984, 0.380935, 0.477464, 0.284404} } }
```

normal SP1 ENERGY 7.9023148559

```
iMinXX2 = {3.2533726279, 6.29961945695, 9.3758871261, 12.50893527675,
  15.6048184074, 18.77126521525, 21.8894836949, 25.07566325} +
  0.000111 * {0.8412609923560835, 0.34846171252933766,
    0.3484617125293, 0.1443375672974, 0.1443375672974,
    0.05978657793452, 0.059786577934523, 0.02476441142835} -
  2.0111 * {-0.27481205092971683, -0.027756838726255537,
    0.18873801105732, 0.23555795315444, 0.5417279059023,
    0.3608860908021, 0.5773809405856, 0.2748120509297}
{3.80614, 6.35548, 8.99635, 12.0352, 14.5154, 18.0455, 20.7283, 24.523}
```

Setxx = iMinXX2

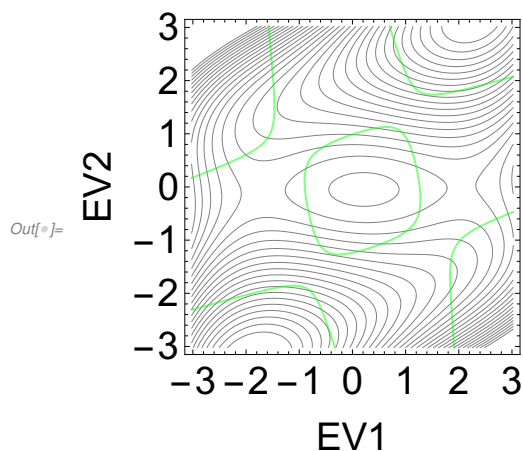
```
SetX = {3.7149759206738477, 6.314091243551704,
  8.944107582930554, 12.036497615782466, 14.623463889232184,
  18.094499719879753, 20.880205952883234, 24.562029621411465}
```

**Eigensystem**

```
{ {4.10197, 3.71954, 3.22835, 2.36292, 1.03721, 0.463518, -0.281982, 0.162696},
  { {-0.0957921, 0.377616, -0.320509, 0.580273, -0.398505,
    0.443616, -0.210905, 0.093302}, {-0.180453, 0.642343,
    -0.282043, 0.0927239, 0.20261, -0.53581, 0.328541, -0.17494},
  {0.168824, -0.518022, -0.050288, 0.624383, -0.177909, -0.322703,
    0.339297, -0.244656}, {0.0454838, -0.100201, -0.109271, 0.236747,
    0.227632, -0.425745, -0.38316, 0.734857}, {0.169415, -0.148624,
    -0.461061, 0.113534, 0.668336, 0.217585, -0.300395, -0.373482},
  {-0.333708, 0.10131, 0.590631, 0.28248, 0.0871379, -0.189319,
    -0.51589, -0.374377}, {0.828543, 0.366142, 0.372955, 0.154241,
    0.11211, 0.0491965, 0.0359823, 0.0169448}, {-0.318032, 0.000879714,
    0.320528, 0.30382, 0.49984, 0.380935, 0.477464, 0.284404} } }
```

Energy 7.9023148559

```
ConSummit = ContourPlot[plane[s, a], {s, -3.0253, 3.0253},
  {a, -3.0253, 3.0253}, FrameLabel → {"EV1", "EV2"},
  Contours → 33, PlotPoints → 79, ContourShading → False,
  ContourStyle → Thickness[0.0015], FrameStyle → Directive[20]]
p1[s_, a_] = D[plane[s, a], s]
p3[s_, a_] = D[plane[s, a], a]
p33[s_, a_] = D[p3[s, a], a]
p31[s_, a_] = D[p3[s, a], s]
p11[s_, a_] = D[p1[s, a], s]
DetH[s_, a_] = p11[s, a] * p33[s, a] - p31[s, a] * p31[s, a]
deter1 = ContourPlot[
  Evaluate[DetH[s, a], {s, -3.04, 3.04}, {a, -3.04, 3.04}, ContourShading → False,
    PlotPoints → 40, Contours → {0.0}, ContourStyle → {Thickness[0.006], Green}]]
Show[ConSummit, deter1]
```

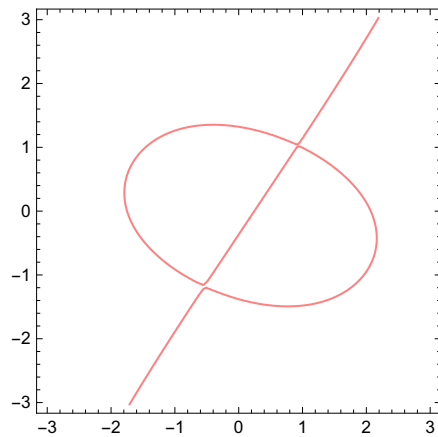


```

congr11 = ContourPlot[p1[s, a], {s, -3.04, 3.04}, {a, -3.04, 3.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Thickness[0.004]}]
congr33 = ContourPlot[p3[s, a], {s, -3.04, 3.04}, {a, -3.04, 3.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Thickness[0.004]}]
congr13 = ContourPlot[-p1[s, a] + p3[s, a], {s, -3.04, 3.04}, {a, -3.04, 3.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Black, Thickness[0.00777]}]

conX = ContourPlot[p1[s, a] - 0.1625 * p3[s, a], {s, -3.04, 3.04}, {a, -3.04, 3.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Thickness[0.005], Red}]

```



```

BildSP2 = Show[ConSummit, conX, congr11, congr33, congr13, deter1, xxSummit]

```

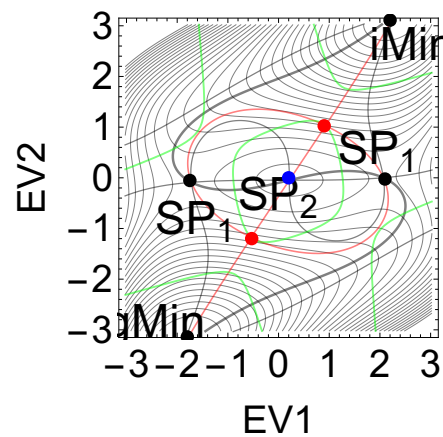


Bild TILTING

as = 6.283185307180

PlaX = {3.2533726279, 6.29961945695, 9.3758871261, 12.50893527675,  
15.6048184074, 18.77126521525, 21.88948369495, 25.075663252}

+ a \* {0.8412609923560835, 0.34846171252933766, 0.3484617125293367,  
0.14433756729740574, 0.14433756729740468, 0.05978657793452398,  
0.059786577934523494, 0.02476441142835576}

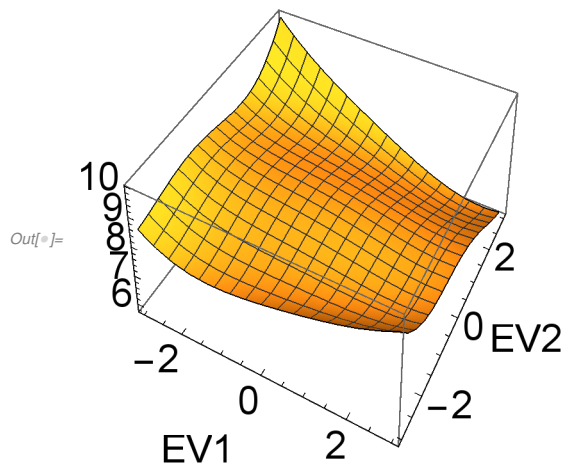
+ s \* {-0.27481205092971683, -0.027756838726255537,  
0.188738011057324, 0.235557953154444, 0.5417279059023,  
0.3608860908021146, 0.57738094058568, 0.27481205092971}

note : a - EV ist non - sym, not a - sym !!!

a0 = 0.5 \* as

k = 1.0

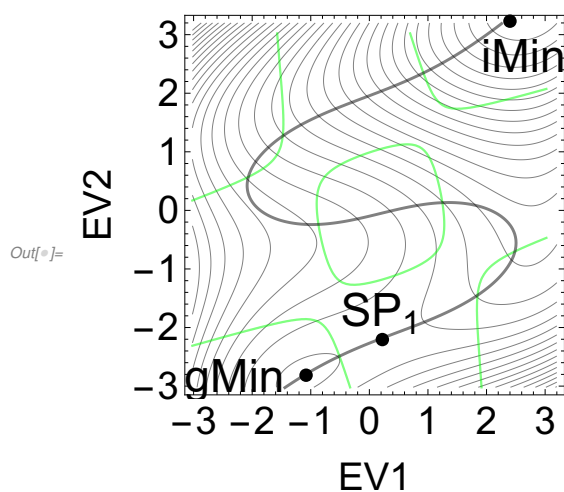
planeT[s\_, a\_] = Sum[1 - Cos[PlaX[[i]]], {i, 8}] +  
Sum[k/2. \* (PlaX[[i + 1]] - PlaX[[i]] - a0)^2, {i, 7}] - 0.2 \* (s + a)



In[ ]:= congr13 = ContourPlot[-p1[s, a] + p3[s, a], {s, -3.04, 3.204}, {a, -3.04, 3.204},  
ContourShading -> False, PlotPoints -> 55,  
Contours -> {0.0}, ContourStyle -> {Black, Thickness[0.00777]}]

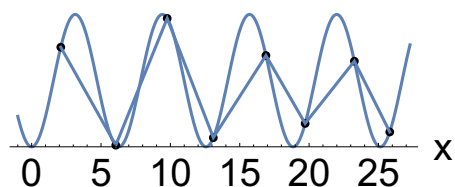
ConSummitT = ContourPlot[planeT[s, a],  
{s, -3.02, 3.2}, {a, -3.02, 3.2}, FrameLabel -> {"EV1", "EV2"},  
Contours -> 33, PlotPoints -> 79, ContourShading -> False,  
ContourStyle -> Thickness[0.0015], FrameStyle -> Directive[20]]

```
BildTilt = Show[ConSummitT, deter1, congr13, xxSummitT]
```



```
start energy 6.60797599 detHess 20.100
0.761389 × 4.59291 × 7.43156 × 11.1823
13.9504 × 17.70120 × 20.53980 × 24.3714
```

```
SP1 node89 energy = 7.8981150 detHess - 1.921546
node89 = {2.1002103793, 6.0642690909, 9.7705188886,
13.0972377523, 16.8896008593, 19.7160983119,
23.2640534983, 25.8154141029}
SetX = node89
```



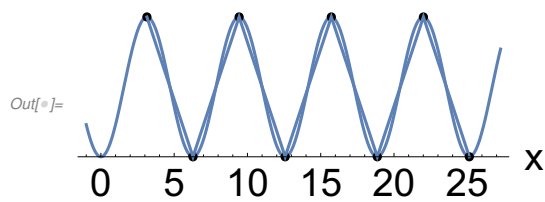
SP1 is already ' over the top ' ! To SP2 it goes back !  
from SP1 the MEP ok down to aim



```

SP2 node126 energy = 7.9983020009 detHess 0.9902674
node126 = {3.1400544682, 6.2847214351, 9.4324606578,
12.5740533870, 15.7248649418, 18.8603117558,
22.0080503250, 25.1404240773}
SP1 node 153 energy = 7.90129220 detHess - 2.399351819
3.7012230186 × 6.3104577282 × 8.9454765206
12.0401697994 × 14.6311263837 × 18.1010605416
20.8889726668 × 24.5675920677
gMin node246 energy = 6.60868238 detHess 20.0730
5.5201586615 × 7.9711863726 × 11.4159006330
13.9482062379 × 17.4632589936 × 19.9958307036
23.4401854848 × 25.8924909560
! only x_1 is  $1 \times 1/2 \text{ Pi}$  moved, not x_8
but at the End ok
node505
7.3604167475 × 11.2818892326 × 14.1432721289
17.9038475873 × 20.7527194939 × 24.4460771508
27.4046836037 × 31.0266179010

```



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

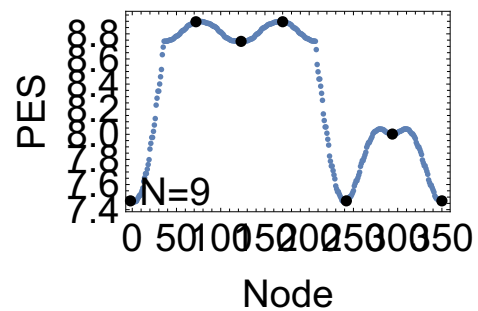
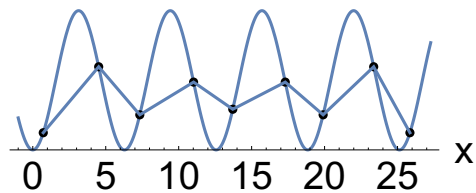
```
Half N = 9 local minimum start a0
```

```
Energy 7.463028576145586
```

```
SetX = {0.7175692976834966, 4.516717261192274, 7.334947933169687,  
11.02147751447118, 13.708342565596421, 17.304662821650844,  
19.90131854752902, 23.36627318273135, 25.85031052640226}
```

```
Eigenvalues
```

```
{4.117285783954124, 3.7597347640309957, 3.1986567467371008,  
2.542766245444331, 2.1556952520213204, 1.3823487864154531,  
0.7857243594195373, 0.3960726621045225, 0.239362228108963}
```



```

SP at node72
energy = 8.89642 detHess - 7.7142 true SP at node77
node72 = {3.8095018322, 6.2716544373, 8.7222764218,
11.8190488528, 14.2361437162, 17.6483444556,
20.1280677344, 23.5653804164, 26.0026988190}
stat point energy = 8.74220 detHess 0.8358861 MIN
node122 = {5.2474601357, 7.5289192156, 10.7580090892,
13.0151851090, 15.7062588727, 18.3990370308,
20.6563824797, 23.8860018717, 26.1676698409}
next SP1 at node 170
node170 = {5.4646190105, 7.8789991556, 11.2930663789,
13.7510589804, 17.1354333411, 19.5300613384,
22.5538752777, 25.0441947839, 27.4460835077}
stat point min 242 energy = 7.4651082 detHess 27.3634
node242 = {5.5678477826, 8.0515087957, 11.5157246667,
14.1121960883, 17.7083557543, 20.3953813954,
24.0820952811, 26.9010647172, 30.7005890113}
node294 energy = 8.00193 detHess 3.725 E - 004
? BBP point crossed ?
node294 = {6.2955518485, 9.4247485813, 12.5539746939,
15.6708052017, 18.8247852320, 21.9539971059,
25.1203519069, 28.2743177017, 31.4282996767}
next min node351 energy = 7.465805 detHess 28.56366
node351 = {7.0176474526, 10.8138655748, 13.6265473505,
17.3116709963, 19.9973361734, 23.5948563035,
26.1929179649, 29.6634214964, 32.1503886813}

Half N = 9 global iMinimum Mirror to a0 Min
Setxx = node242

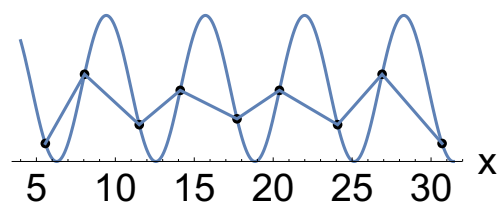
Energy 7.463028576145592

SetX = {5.56561600949567, 8.049653353166578, 11.514607988368912,
14.11126371424709, 17.707583970301513, 20.394449021426755,
24.080978602728244, 26.899209274705658, 30.698357238214435}

```

### Eigenvalues

```
{4.11729, 3.75973, 3.19866, 2.54277, 2.1557, 1.38235, 0.785724, 0.396073, 0.239362}
```



```

N = 9 SP at node72 energy = 8.89642 detHess - 7.7142
node72 = {3.8095018322, 6.2716544373, 8.7222764218,
11.8190488528, 14.2361437162, 17.6483444556,
20.1280677344, 23.5653804164, 26.0026988190}
Setxx = node72

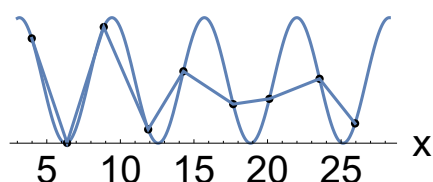
```

```
SetX = {3.9786402294945615, 6.377563639033659, 8.870725333939804,
  11.890024919825066, 14.283377162034082, 17.666059717770544,
  20.12281012393347, 23.53562048473063, 25.9487773129896}
```

Eigenvalues

```
{4.13131, 3.81303, 3.39132, 2.76302,
  1.79884, 0.950864, 0.48346, 0.272214, -0.164738}
```

ENERGY SP1 8.899754095306



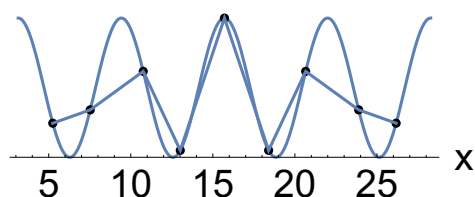
```
stat point energy = 8.74220 detHess 0.8358861 is flat iMin
node122 = {5.2474601357, 7.5289192156, 10.7580090892,
  13.0151851090, 15.7062588727, 18.3990370308,
  20.6563824797, 23.8860018717, 26.1676698409}
Setxx = node122
```

Energy 8.7413204660647

```
SetX = {5.2478583979904, 7.529421935729, 10.758776695236,
  13.016037201528, 15.707963074264, 18.399889132613,
  20.657149694346, 23.886504443703, 26.16806796394}
```

Eigenvalues

```
{4.13577, 3.81053, 3.21935, 2.95419,
  1.5395, 1.33618, 0.590946, 0.394235, 0.0095686}
```



```
node294 energy = 8.00193 detHess 3.7250869344633715 E - 004
? BBP point crossed
node294 = {6.2955518485, 9.4247485813, 12.5539746939,
  15.6708052017, 18.8247852320, 21.9539971059,
  25.1203519069, 28.2743177017, 31.4282996767}
Setxx = node294
```

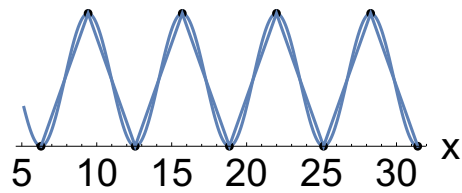
```
SetX = {6.2827412826258, 9.423889911707, 12.565926589797,
  15.70751924337106, 18.84955592153876, 21.991592599706,
  25.133185253280068, 28.2752219313708, 31.4163705604516}
```

Energy 8.0

**Eigenvalues**

$\{4.12269, 3.80194, 3.34168, 2.44504,$   
 $2.38589, 0.753021, 0.332652, -0.182913, 2.1124 \times 10^{-7}\}$

SP  $1 \times 1/2$



```
### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

Half N = 9 global SP start a0

```
Setxx = Table[a0 * (i - 1) + Pi, {i, 9}]
```

```
{3.141592653589793, 6.283185307179793, 9.424777960769793,  
12.566370614359794, 15.707963267949793, 18.849555921539793,  
21.991148575129795, 25.132741228719794, 28.274333882309794`}
```

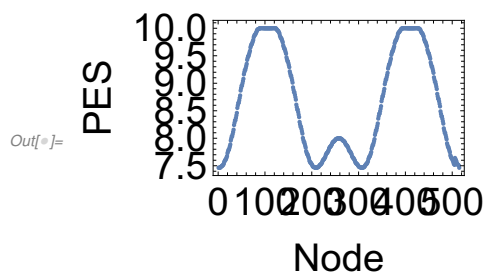
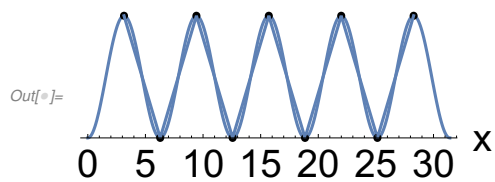
```
SetX = {3.14149036861906, 6.2831853071799, 9.424880245741,  
12.5664728993304, 15.7081678378905, 18.8496582065098,  
21.9912508600997, 25.132741228718, 28.2742315973367}
```

**Eigenvalues**

Out[8]=  $\{4.13452, 3.85381, 3.47192, 3.13317,$   
 $0.818906, -0.425345, 0.413551, -0.400523, 9.41599 \times 10^{-9}\}$

Energy 10.0

SP  $2 \times 1/2$



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

```
Half N = 10 global minimum start a0
```

```
Energy 8.354573773374055
```

```
SetX = {-0.745405090457349,
```

```
1.7179180566566765, 5.1704382836780685, 7.726041843300373,
```

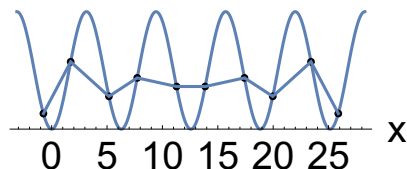
```
11.273472281584192, 13.859268545497727, 17.406698978202854,
```

```
19.962302551388554, 23.414822828329495, 25.878146105816462}
```

```
Eigenvalues
```

```
{4.14073, 3.84907, 3.38728, 2.79254,
```

```
2.34474, 1.84356, 1.1821, 0.695723, 0.377502, 0.25145}
```



```
stat points SP1 energy = 9.70709 detHess - 7.0989
```

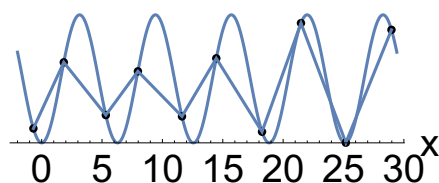
```
node73 = {-0.6836948031, 1.8322587064, 5.3142252123,
```

```
7.9718943086, 11.6226197566, 14.4635805791,
```

```
18.2517397944, 21.4770603094, 25.1941219932,
```

```
28.9725259057}
```

```
SetX = node73
```



```
sp1Half
```

```
Min energy = 8.354758 detHess 46.56279
```

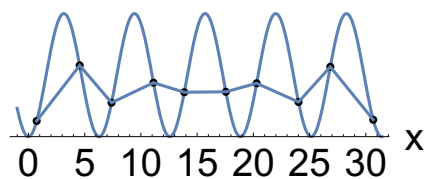
```
node406 = {0.7314473908, 4.5541861648, 7.3894129258,
```

```
11.1186545703, 13.8554610357, 17.5528501047,
```

```
20.2875674049, 24.0134817435, 26.8396185161,
```

```
30.6565105541}
```

```
SetX = node406
```



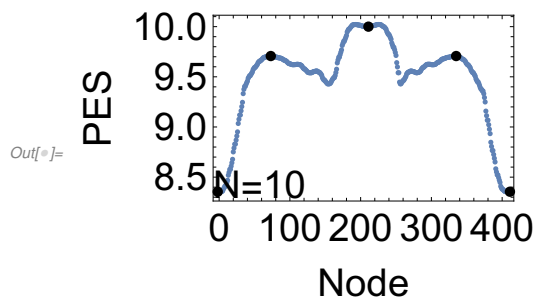
```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

```
N = 10 Half
```

```

stat points SP1 energy = 9.70709 detHess - 7.0989
node73 = {-0.6836948031, 1.8322587064, 5.3142252123,
7.9718943086, 11.6226197566, 14.4635805791,
18.2517397944, 21.4770603094, 25.1941219932,
28.9725259057}
energy = 10.000002 detHess 0.99 SP2
node211 = {0.0028938010, 3.1459333329, 6.2846321976,
9.4247779524, 12.5649237169, 15.7036225836,
18.8466621244, 21.9868078719, 25.1312943092,
28.2743338272}
SP1 energy 9.70707 detHess - 7.512
node335 = {0.6857801967, 4.4524119879, 7.2526478865,
10.8774655756, 13.5092499944, 16.9502873874,
19.4447884707, 22.4999908784, 25.0680267397,
27.5713932727}
Min energy = 8.354758 detHess 46.56
node406 = {0.7314473908, 4.5541861648, 7.3894129258,
11.1186545703, 13.8554610357, 17.5528501047,
20.2875674049, 24.0134817435, 26.8396185161,
30.6565105541}

```



```

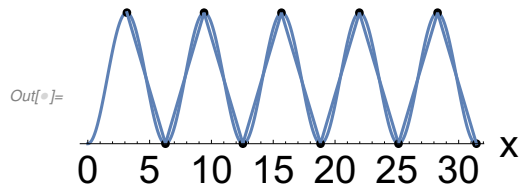
Half N = 10 global SP start a0 + Pi
as = 6.283185307180
a0 = as / 2.0
Setxx = Table[a0 * (i - 1) + Pi, {i, 10}]
Out[ ]= {3.14159, 6.28319, 9.42478, 12.5664,
15.708, 18.8496, 21.9911, 25.1327, 28.2743, 31.4159}

SetX = {3.1626043096532723,
6.283186853217254, 9.403770942818902, 12.545360505357145,
15.665941504589348, 18.828531901067812, 21.970099825843672,
25.132714945664652, 28.295303782431947, 31.43692425591413}

```

## Eigenvalues

Out[ ]= {4.14897, 3.90212, 3.54338, 3.17544, 2.41409,  
0.824871, 0.45679, -0.414017, -0.148728, 0.0981828}



Energy 10.00022058998119

## ## ## ## ## ## ## ## ## ## ## #

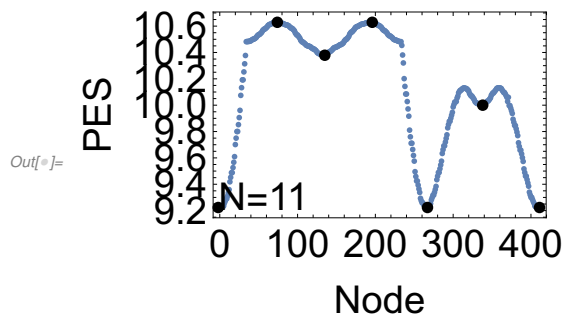
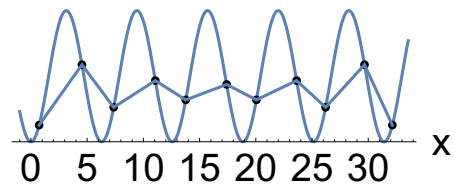
Half N = 11 global minimum start a0

Energy 9.223516708398785

SetX = {0.728681832579204, 4.536161307779916,  
7.35912868115826, 11.062134584978912, 13.767354880664323,  
17.404970575488314, 20.050540307754943, 23.628505301370836,  
26.208684621357346, 29.6689025462588, 32.144608438232545}

## Eigenvalues

{4.15803, 3.91652, 3.53147, 3.0258, 2.50325,  
2.16888, 1.55243, 1.0155, 0.611273, 0.346896, 0.243012}





```

stat point node74 SP
energy = 10.3790359 detHess 9.8739820 is IMin
node135 = {5.3767666679, 7.7222204262, 11.0590062277,
13.3978031603, 16.4754974971, 18.8588289129,
21.2514331871, 24.3181151687, 26.6573280761,
29.9954735156, 32.3448992384}
energy = 10.629015 SP1 detHess - 16.777
node196 = {5.5089457769, 7.9592017306, 11.4039271553,
13.9308764392, 17.4366231886, 19.9548045396,
23.3665617169, 25.7973455452, 28.8448770878,
31.3523193361, 33.7961972671}
Min energy = 9.223548 detHess 75.997
node267 = {5.5487151759, 8.0255873265, 11.4877713187,
14.0686585607, 17.6472000213, 20.2928513044,
23.9303853477, 26.6350292206, 30.3373273151,
33.1583286948, 36.9646418923}
energy = 10.0000272 detHess 0.9986 SP2
node338 = {6.2779648295, 9.4195578714, 12.5663709789,
15.7131844511, 18.8547767638, 22.0015898951,
25.1379618961, 28.2795545409, 31.4159265508,
34.5522985755, 37.6938911905}
energy = 9.223524 detHess 77.242976
node410 = {7.0090224564, 10.8170695891, 13.6410064258,
17.3443600984, 20.0498647125, 23.6875202609,
26.3330500390, 29.9107307584, 32.4905624223,
35.9498109578, 38.4249491724}
SP by node74 Energy at pes 10.6290626

node74 = {3.9014847740, 6.3560131461, 8.8716824878,
11.9209833917, 14.3518304878, 17.7622096058,
20.2775400043, 23.7728276074, 26.2971863199,
29.7291990437, 32.1692223723}
Setxx = node74

SetX = {3.924096304054047, 6.360631865463567,
8.874536588024338, 11.911334300471788, 14.338943971338324,
17.746265631389914, 20.260892295328297, 23.762832137994014,
26.284882055139985, 29.720568320924187, 32.22780628178085}

```

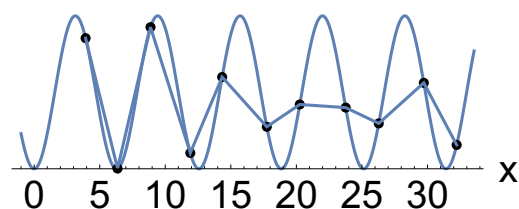
#### Eigenvalues

```

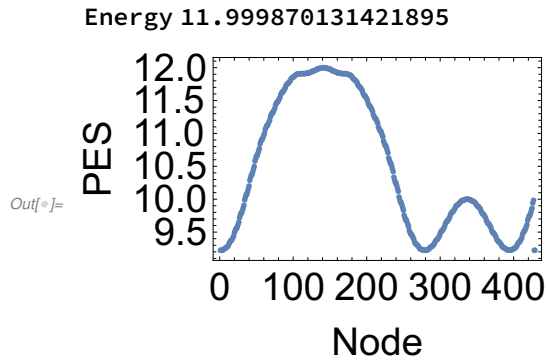
{4.166, 3.94349, 3.61381, 3.22599, 2.6366,
1.91511, 1.16842, 0.696629, 0.382214, 0.248554, -0.189338}

```

SP ENERGY 10.631582760474







```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

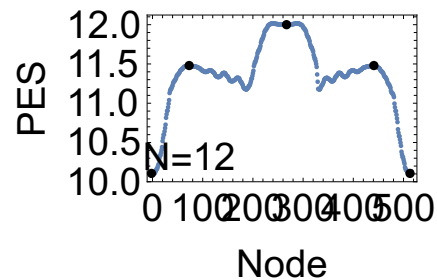
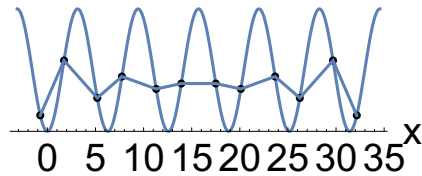
```
Half N = 12 global minimum start a0
```

```
Energy 10.106299448564279
```

```
SetX = {-0.7391303202425, 1.7288169075135, 5.184304843658, 7.749093795169,
 11.308387058759, 13.91620857867, 17.499717956736, 20.10753947656,
 23.666832739816, 26.23162169118, 29.687109626319, 32.15505685511}
```

```
Eigenvalues
```

```
{4.17123, 3.96756, 3.64078, 3.20793, 2.70299, 2.33504,
 1.9184, 1.35271, 0.900304, 0.557341, 0.33418, 0.247295}
```



```
SP 1
```

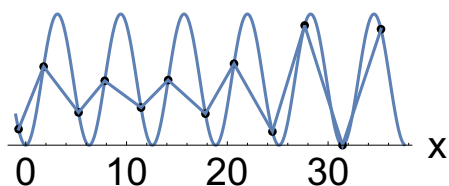
```
stat points energy = 11.479833 detHess - 20.71 SP1
node73 = {-0.7074454423, 1.7773540918, 5.2408963135,
 7.8408778332, 11.4407734999, 14.1381442716,
 17.8355145662, 20.6839104992, 24.4977755375,
 27.7184906829, 31.4668655767, 35.2661574847}
Setxx = node73
```

```
SetX = {-0.715450709187, 1.77018426684619, 5.236007234679, 7.8358145382397,
 11.4354568246554, 14.130297422004, 17.825114424299, 20.665507288569,
 24.47599986016362, 27.675953123997, 31.433798661677, 35.25020621837}
```

```
Eigenvalues
```

```
{4.17732, 3.98984, 3.70178, 3.35782, 2.91259, 2.32013,
 1.54947, 1.0034, 0.615082, 0.346619, 0.230984, -0.224486}
```

SP 1 ENERGY 11.480016285321586



```
stat points energy = 11.479833 detHess - 20.71 SP1
node73 = {-0.7074454423, 1.7773540918, 5.2408963135,
7.8408778332, 11.4407734999, 14.1381442716,
17.8355145662, 20.6839104992, 24.4977755375,
27.7184906829, 31.4668655767, 35.2661574847}
```

```
flat SP2 energy = 12.00000001 detHess 3.94 E - 002
node267 = {0.0093352365, 3.1602608224, 6.2925193238,
9.4341117063, 12.5663704788, 15.6986291158,
18.8402217693, 21.9724804063, 25.1234061278,
28.2649968839, 31.4159245028, 34.5668500885}
```

```
SP1 energy = 11.479851 detHess - 21.42
node441 = {0.7186765564, 4.5143680775, 7.3296017546,
11.0104700193, 13.6914492234, 17.2747299131,
19.8580187221, 23.2873207994, 25.7540956732,
28.8030075276, 31.3475308733, 33.8237118693}
```

```
Min energy = 10.10655 detHess 117.94
node513 = {0.7554082693, 4.5670971956, 7.3893224189,
11.1055219716, 13.8277596846, 17.5025116216,
20.2021917800, 23.8781691766, 26.6037302073,
30.3243146179, 33.1575277776, 36.9761892076}
```

SP 2

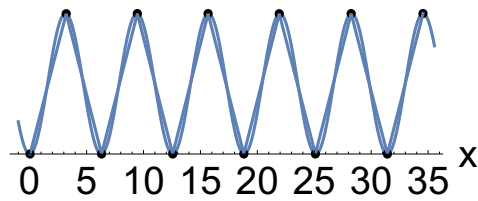
```
flat SP2 energy = 12.00000001 detHess 3.94 E - 002
node267 = {0.0093352365, 3.1602608224, 6.2925193238,
9.4341117063, 12.5663704788, 15.6986291158,
18.8402217693, 21.9724804063, 25.1234061278,
28.2649968839, 31.4159245028, 34.5668500885}
```

Setxx = node267

SetX = {0.03445496266684, 3.210495762159, 6.317687961314, 9.459375969495, 12.566472870968, 15.673672029049, 18.81515570598, 21.922245951665, 25.098184313735, 28.239572638277, 31.421999455569, 34.55002809979}

## Eigenvalues

```
{4.1753575238268645, 3.9999924807730216, 3.731975622757413,
 3.4142591734846413, 3.125714011250758, 2.414023430379269,
 0.8750560405314829, 0.586546645740515, -0.414085376729246,
 0.268764956327468, -0.17458678742619, 0.0011507374089987}
```



```
Setxx = {-0.5005178209147, 2.04896293431, 5.489190189184383, 7.994878187742478,
 11.68264539868323, 14.3411199219025, 18.1541000403284, 21.17772072683093,
 24.93392485817119, 28.5138140323775, 32.031924385664, 36.3355047436099}
```

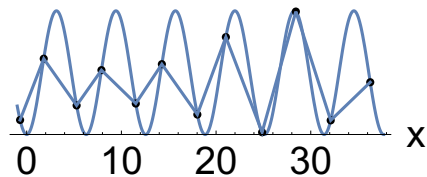
becomes

```
SetX = {-0.699172111306, 1.798836279946, 5.270956042237374, 7.895060406648561,
 11.51832115691837, 14.275130864589622, 18.0224386362198, 21.033763574425887,
 24.862777527376632, 28.425095027404694, 32.1058123917316, 36.283481740713974}
```

**Eigenvalues**

```
{4.17603, 3.97961, 3.66993, 3.34264, 2.98025, 2.32922,
 1.4523, 1.02089, 0.772981, 0.439473, 0.252619, -0.0236753}
```

SP1 ENERGY 11.39214381256 is new point



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

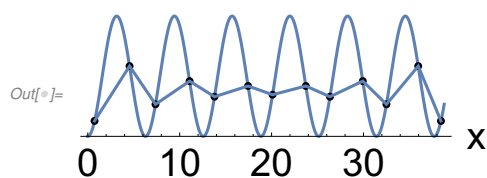
N = 13 HALF global minimum start a0

Energy 10.98053863617295

```
SetX = {0.7327678900185, 4.543290165719, 7.36807568108,
 11.0771134709, 13.7894738108559, 17.4419953714012, 20.107810464839,
 23.725180707792, 26.3558444056255, 29.9266693654348,
 32.50081682802, 35.959216559529, 38.43187962525977}
```

**Eigenvalues**

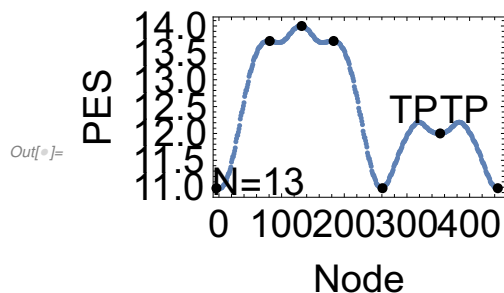
```
Out[ ]= {4.18145, 4.00766, 3.7274, 3.3538, 2.90441, 2.47492,
 2.17796, 1.66986, 1.19068, 0.802807, 0.508423, 0.317689, 0.243888}
```



```

SP2 node81 energy = 13.7207373 detHess 5.711
3.8295789768 × 6.3429387994 × 8.9160165624
11.9761902153 × 14.4798529535 × 17.9253712076
20.5727596313 × 24.2085565148 × 27.0462235679
30.8257461368 × 34.0487577908 × 37.7588653350
41.5286908195
sp 3 node132 energy = 13.99977320 detHess - 0.9997792
3.1397806993 × 6.2822793305 × 9.4238719852
12.5663706154 × 15.7088692465 × 18.8504618992
21.9929605294 × 25.1336472064 × 28.2752398608
31.4159265369 × 34.5566132139 × 37.6982058664
40.8388925424
SP node183 energy = 13.72103154 detHess 7.125657
2.4589018869 × 6.2275477778 × 9.9405848395
13.1603849919 × 16.9398773848 × 19.7762429323
23.4122434076 × 26.0594282395 × 29.5062479992
32.0099409135 × 35.0733260685 × 37.6434743139
40.1580137304
Min node 261 energy = 10.9813521 detHess 200.62
5.5428512077 × 8.0171263815 × 11.4781229423
14.0533043756 × 17.6249714050 × 20.2559735027
23.8734958098 × 26.5391588098 × 30.1913420193
32.9028602970 × 36.6108641709 × 39.4330529173
43.2419630507
node353 energy = 12.00037527 detHess 1.003
6.2829065280 × 9.4243597921 × 12.5662312248
15.7079632680 × 18.8496953111 × 21.9915667439
25.1330200079 × 28.2747520510 × 31.4160659255
34.5575191895 × 37.6989724535 × 40.8402863280
43.9820183711
Min node 445 energy = 11.10873637 detHess 187.18887
7.3627475483 × 11.0781491085 × 13.7969580324
17.4584519330 × 20.1360471066 × 23.7734990663
26.4332452725 × 30.0566843737 × 32.7024177211
36.3080078548 × 38.9296992614 × 42.4940756446
45.0618593916

```



```

start min
{0.7327678900184654, 4.543290165719971, 7.36807568108211,
 11.0771134707699, 13.789473810855899, 17.441995371401205,
 20.10781046483944, 23.72518070779202, 26.355844405625465,
 29.926669365434876, 32.5008168280212, 35.95921655952915, 38.43187962525977}
SP node58 energy = 12.37472065 detHess - 37.07
3.8914549258 × 6.3472329262 × 8.8670147664
11.9160863324 × 14.3597452047 × 17.7787356308
20.3201320063 × 23.8565105379 × 26.4359607294
29.9798253250 × 32.5327475967 × 35.9843807570
38.4463546474
Imin node128 energy = 12.06875169 detHess - 0.408366
? BBP point crossed ?
 5.4253847791 7.8105628443 × 11.1947984620
13.5988136639 × 16.8613830235 × 19.2097968553
21.9107103992 × 24.6919754039 × 27.0466081873
30.3429671774 × 32.7607086468 × 36.1530174458
38.5456313218
374 energy = 12.3758001 detHess - 40.97449039
5.5402384845 × 8.0011290509 × 11.4512129565
14.0033166879 × 17.5464758404 × 20.1252574613
23.6608136617 × 26.2012533981 × 29.6181783245
32.0607464783 × 35.1043691770 × 37.6279926984
40.0805570125
node428 energy = 13.72008833 detHess 6.4740
2.4667023382 × 6.2335128769 × 9.9506714094
13.1658440149 × 16.9452243941 × 19.7797138962
23.4159177718 × 26.0627646760 × 29.5112455385
32.0149499928 × 35.0824906758 × 37.6488430278
40.1649477331
node492 energy = 13.9983833979 detHess - 1.00032
3.1446267373 × 6.2862192426 × 9.4308456789
12.5694044340 × 15.7109970042 × 18.8495558428
21.9881146025 × 25.1297073303 × 28.2682661643
31.4128926792 × 34.5544853420 × 37.6991118477
40.8437383579

```

next calculation

SP node76 energy = 12.37447999 detHess - 40.245

5.5357293864 × 7.9975469578 × 11.4490767209  
 14.0016883393 × 17.5451367629 × 20.1238542936  
 23.6589373785 × 26.1987205471 × 29.6137667082  
 32.0554582268 × 35.0939694927 × 37.6213926054  
 40.0711746977

gMin node131 energy = 10.98154004 detHess 198.09

5.5503348611 × 8.0229365119 × 11.4812992139  
 14.0553251658 × 17.6260039531 × 20.2563686912  
 23.8733182294 × 26.5383540407 × 30.1897780485  
 32.9000075623 × 36.6064796602 × 39.4251105705  
 43.2317217446

node224 energy = 11.79733153 detHess - 4.49

5.7008992936 × 8.2925572790 × 11.7895726986  
 14.5855887057 × 18.2827371715 × 21.4429346120  
 25.1242958084 × 28.7972116849 × 31.9707520722  
 35.6710874749 × 38.4741432184 × 41.9769374521  
 44.5726777301

node274 energy = 11.99950482 detHess 1.00315585

6.2801088149 × 9.4186249810 × 12.5632940881  
 15.7048866739 × 18.8495558488 × 21.9942249511  
 25.1358176823 × 28.2804868621 × 31.4190031009  
 34.5605959000 × 37.6991119934 × 40.8376282371  
 43.9792207355

node321 energy = 11.7972555 detHess - 4.7448

6.8644188215 × 10.5550667834 × 13.3411793646  
 16.8268713755 × 19.4129391991 × 22.5330566742  
 25.1374025014 × 27.7464095845 × 30.8591579905  
 33.4434608336 × 36.9252595760 × 39.7081626681  
 43.3965595230

node413 energy = 10.98254327 detHess 213.43

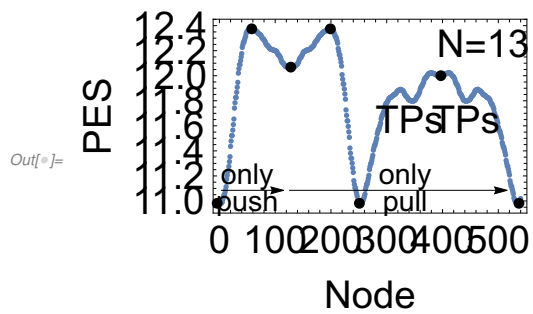
7.0159929361 × 10.8265447686 × 13.6513481102  
 17.3604443592 × 20.0728749539 × 23.7255403016  
 26.3915575582 × 30.0093025031 × 32.6404934779  
 36.2123434205 × 38.7877216304 × 42.2490829451  
 44.7236050738

node468 energy = 12.374175 detHess - 35.92779

7.0305882521 × 10.8519171352 × 13.6835469732  
 17.4140434571 × 20.1536768548 × 23.8579625983  
 26.6057425796 × 30.3487444429 × 33.2159022281  
 37.0569131668 × 40.2989665602 × 44.566458112  
 47.8886052456



profilGesamtPushandPull



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

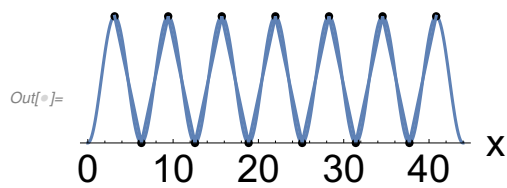
```
N = 13 HALF global SP start a0 + Pi
```

```
Setxx = Table[a0 * (i - 1) + Pi, {i, 13}]
```

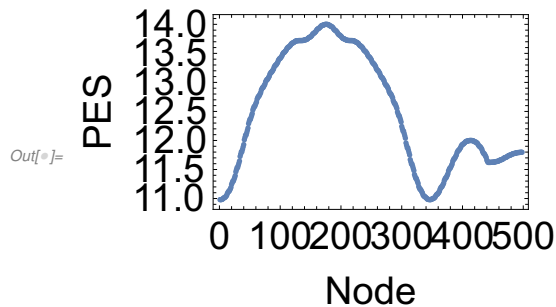
```
SetX = {3.14159265358979, 6.28318530717979, 9.424777960769998,  
12.566370614359586, 15.707963267949586, 18.849555921538965,  
21.991148575128552, 25.13274122871814, 28.274333882307516,  
31.415926535897515, 34.5575191894871, 37.69911184307731, 40.84070449666731}
```

Eigenvalues

```
Out[ ] = {4.18611, 4.04153, 3.81887, 3.54838, 3.27843, 3.0753, 0.904247,  
0.66397, -0.416251, -0.412061, 0.366792, -0.138206, 0.0828754}
```



Energy 14.0



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

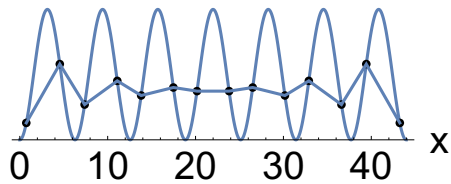
```
N = 14 HALF: global minimum start a0
```

```
ENERGY 11.86002431625168
```

```
SetX = {0.7367105244197749, 4.550158307312402, 7.376736587333729,  
11.091578629317983, 13.811025564449617, 17.4777580919862, 20.16422559674096,  
23.818071543932472, 26.504539047203448, 30.171271618140672,  
32.890718517057486, 36.6055605169502, 39.432138807263826, 43.24558658145119}
```

```
Eigenvalues
```

```
{4.18959, 4.03944, 3.79627, 3.47024, 3.07403, 2.64131, 2.32708,  
1.96898, 1.48074, 1.0669, 0.72929, 0.473567, 0.308755, 0.245319}
```



```
stat points detHess - 52.96 SP1
```

```
node74 = {3.8612362680, 6.3355487355, 8.8622007051,  
11.9222206991, 14.3817217743, 17.8114680563,  
20.3797796485, 23.9472682856, 26.5880799882,  
30.222338668, 32.9266526939, 36.6292678509,  
39.4547574174, 43.2632109538}
```

```
detHess 2.187 SP2
```

```
node294 = {2.7026318915, 6.2704770854, 9.8256143997,  
12.9905630967, 16.5670967612, 19.3863534887,  
22.7169968218, 25.3838700387, 28.2992407750,  
31.1897071937, 33.8558788089, 37.1675218763,  
39.9722604075, 43.5403236583}
```

```
detHess - 0.986 SP3
```

```
node323 = {3.1507371778, 6.2862332995, 9.4247774088,  
12.5633220701, 15.6988181918, 18.8434592622,  
21.9820037110, 25.1296928966, 28.2743337549,  
31.4189747405, 34.5666639262, 37.7052085024,  
40.8498497002, 43.9853458218}
```

```
SP2
```

```
node349 = {3.5806764595, 6.2960452984, 9.0242737740,  
12.1423849292, 14.8490995946, 18.3129149518,  
21.2654782818, 24.8816786196, 28.2494455629,  
31.6420982562, 35.2589993444, 38.2305513665,  
41.7088782366, 44.4240550646}
```

```
SP1 detHess - 65.093
```

```
node562 = {2.3905687156, 6.2090050292, 9.9533290782,  
13.1933704223, 17.0201296388, 19.8801475725,  
23.5977689385, 26.3160319166, 29.9601494035,  
32.6108743088, 36.1917956990, 38.7747312795,  
42.2375515276, 44.7154628442}
```

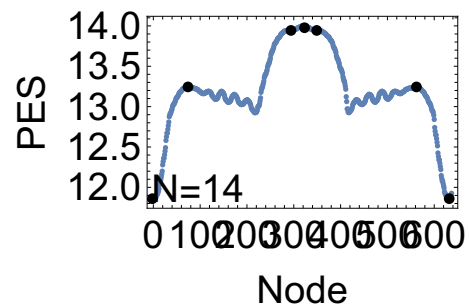
```
min detHess 340.741
```

```
node632 = {5.5470704327, 8.0166789215, 11.4730813761,
```

```
14.0413404906, 17.6050117630, 20.2214328802,
23.8181346914, 26.4474740106, 30.0442078040,
32.6606921829, 36.2244976797, 38.7929251156,
42.2497365981, 44.7196034066}
```

```
node702 = {5.5630430332, 8.0380099433, 11.4960913791,
14.0768382772, 17.6557659533, 20.3049227539,
23.9474249641, 26.6633091401, 30.3783842625,
33.2323019122, 37.0562162720, 40.2806151720,
44.0362759486, 47.8458893142}
```

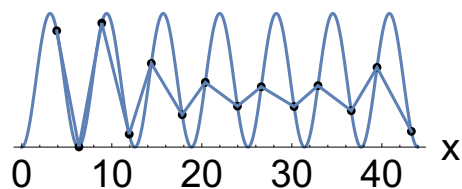
```
node924 = {5.8347893342, 8.5483191286, 12.0303267150,
15.0015955061, 18.6219392235, 22.0166266036,
25.3858387116, 29.0054547768, 31.9573663641,
35.4246483629, 38.1294557570, 41.2514465347,
43.9741475557, 46.6886990725}
```



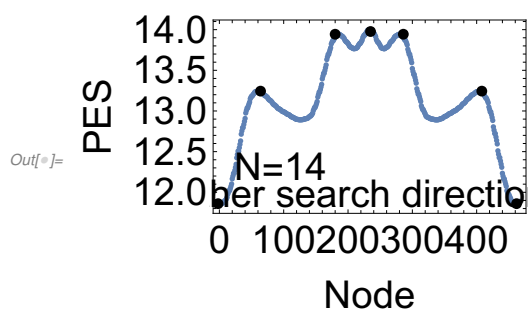
```
N = 14 SP1 halb stat points detHess - 52.96 SP1
node74 = {3.8612362680, 6.3355487355, 8.8622007051,
11.9222206991, 14.3817217743, 17.8114680563,
20.3797796485, 23.9472682856, 26.5880799882,
30.222338668, 32.9266526939, 36.6292678509,
39.4547574174, 43.2632109538}
Setxx = node74
```

```
SetX = {3.8773503069750634, 6.347793946870785,
8.882801286785774, 11.933639023259742, 14.393127001763439,
17.82003565915667, 20.389892403971068, 23.959285283592425,
26.606584723862913, 30.249187918747943, 32.90650168126254,
36.60084246352985, 39.4640282628328, 43.28142676454691}
```

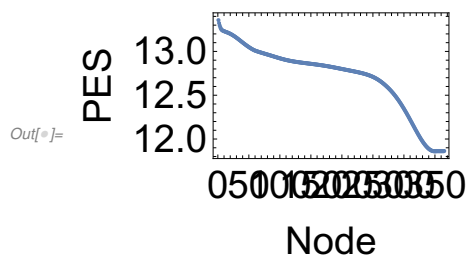
```
SP1halb ENERGY 13.244005784918382
```



NT ueber SP1 rs = EV of SP1 ok !



crosses the SP3 but SD directly down to next Minimum



IRC point energy 11.8636546711 detH 193.12

```
node691 = {5.5461054837536361, 8.0171186574027260, 11.471053617897601,
14.043315215340881, 17.602157545798651, 20.224329346899534,
23.814890011119207, 26.450592446317486, 30.041153110537152,
32.663324911638043, 36.222167242095807, 38.794428839539094,
42.248363800033964, 44.719376973683055}
```

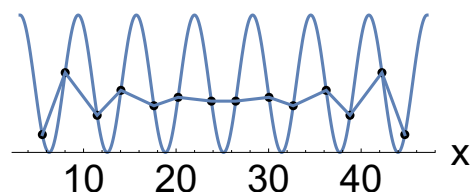
Setxx = node691

```
SetX = {5.546474788537966, 8.016212352802752, 11.472819350341702,
14.041162620072576, 17.604901013464225, 20.22135376270467,
23.81807156842441, 26.44741088901228, 30.04412869473202, 32.66058144397247,
36.22431983736411, 38.79266310709499, 42.24927010463394, 44.719007668898726}
```

Eigenvalues

```
{4.189594490800495, 4.039444317878215, 3.796273913825952, 3.4702378644774483,
3.0740318512132996, 2.64131443492687, 2.327078339362793, 1.968979526859071,
1.4807432502921505, 1.0669042193109273, 0.7292902875913672,
0.473566891136513, 0.30875457953805585, 0.24531945803506175}
```

iMin ENERGY 11.860024316252



iMin is strong compressed - It is moved by -  
 start  
 $-0.7367153072 \times 1.7330246928 \times 5.1896146928 \times 7.7580146928$   
 $11.3217146928 \times 13.9382146928 \times 17.5349146928 \times 20.1642146928$   
 $23.7609146928 \times 26.3774146928 \times 29.9411146928 \times 32.5095146928$   
 $35.9661146928 \times 38.4358146928$   
 but globMin was with same energy  
 $\{0.73671052441977, 4.550158307312402, 7.37673658733372, 11.091578629317983,$   
 $13.811025564449617, 17.4777580919862, 20.16422559674096,$   
 $23.818071543932472, 26.50453904720344, 30.171271618140672,$   
 $32.890718517057486, 36.605560516950, 39.4321388072638, 43.24558658145119\}$

Min detHess 331.64 energy = 11.8615854

ok it is gMin of a0

node462 =  $\{0.7331596880, 4.5459969491, 7.3735952041,$   
 $11.0890333854, 13.8092717018, 17.4765242428,$   
 $20.1634040132, 23.8175310922, 26.5041806466,$   
 $30.1710450917, 32.8905614818, 36.6054635900,$   
 $39.4320602495, 43.2455409102\}$

N = 14 SP2 half

stat points detHess 2.187 SP2

node294 =  $\{2.7026318915, 6.2704770854, 9.8256143997,$   
 $12.9905630967, 16.5670967612, 19.3863534887,$   
 $22.7169968218, 25.3838700387, 28.2992407750,$   
 $31.1897071937, 33.8558788089, 37.1675218763,$   
 $39.9722604075, 43.5403236583\}$

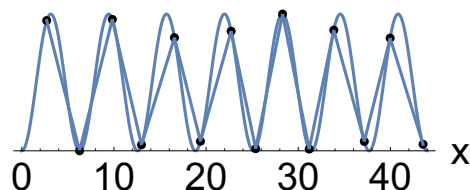
Setxx = node294

SetX =  $\{2.7015370340540885, 6.26911947391867,$   
 $9.822636544333124, 12.988708538953404, 16.564674603392156,$   
 $19.384947847194237, 22.715399252605554, 25.383276268946407,$   
 $28.299075616228208, 31.190135753802092, 33.85731874935583,$   
 $37.168872724274, 39.97468705904758, 43.542256214259034\}$

Eigenvalues

$\{4.195398881695557, 4.061389110870293, 3.8514123872159156, 3.5824524701801854,$   
 $3.3206057194534804, 3.030961737650185, 2.383955961211218, 1.1007305893405146,$   
 $0.8290118042914019, 0.5345581237525465, -0.3330567642474742,$   
 $0.264136572283055, 0.10893590680452991, -0.09038736756580246\}$

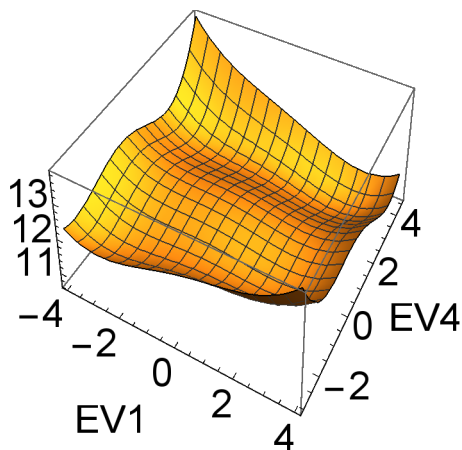
SP2 halb ENERGY 13.94272107209335



```

Search for SP1 near SP2 sym is EV1, asym is EV4
PlaX = {2.7015370340540885, 6.26911947391867,
  9.822636544333124, 12.988708538953404, 16.564674603392156,
  19.384947847194237, 22.715399252605554, 25.383276268946407,
  28.299075616228208, 31.190135753802092, 33.85731874935583,
  37.168872724274, 39.97468705904758, 43.542256214259034} +
a * {0.8377616983371169, 0.358837457055474, 0.35822841817569445,
  0.14668158181076066, 0.11778116916544437, 0.050970595056006124,
  0.044974338049144226, 0.020271484113743122, 0.021958791678807345,
  0.009007552400002634, 0.007835256441641387, 0.0032808228301697464,
  0.0026494099144804715, 0.0011839398432581159} +
s * {-0.11316151099690783, -0.02100949781614423, 0.0482361026527749,
  0.07737312228759498, 0.18407828317506006,
  0.186864100309721, 0.36725604350859486, 0.30576994423246584,
  0.5681453649503583, 0.3139024718374035, 0.39396719955258985,
  0.20836972860450872, 0.22136393062756007, 0.11095260124431998}
note : a - EV ist non - sym, not a - sym !!!
as = 6.283185307180
a0 = 0.5 * as
k = 1.0
plane[s_, a_] = Sum[1 - Cos[PlaX[[i]]], {i, 12}] +
  Sum[k/2. * (PlaX[[i + 1]] - PlaX[[i]] - a0)^2, {i, 11}]
Plot3D[plane[s, a], {s, -4.0253, 4.0253}, {a, -3.0253, 4.50253},
  AxesLabel -> {"EV1", "EV4"}, AxesStyle -> Directive[20], AspectRatio -> 1.111]

```



```

ConSummit = ContourPlot[plane[s, a], {s, -4.0253, 4.0253},
  {a, -4.0253, 4.0253}, FrameLabel -> {"EV1", "EV4"},
  Contours -> 33, PlotPoints -> 79, ContourShading -> False,
  ContourStyle -> Thickness[0.0015], FrameStyle -> Directive[20]]

```

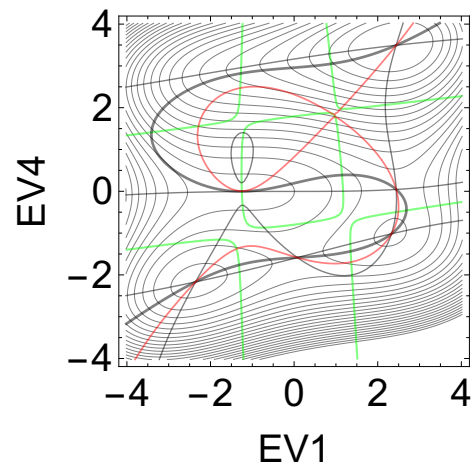
```

p1[s_, a_] = D[plane[s, a], s]
p3[s_, a_] = D[plane[s, a], a]
p33[s_, a_] = D[p3[s, a], a]
p31[s_, a_] = D[p3[s, a], s]
p11[s_, a_] = D[p1[s, a], s]
DetH[s_, a_] = p11[s, a] * p33[s, a] - p31[s, a] * p31[s, a]

deter1 = ContourPlot[Evaluate[DetH[s, a], {s, -4.0253, 4.0253},
  {a, -4.0253, 4.0253}], ContourShading → False, PlotPoints → 40,
  Contours → {0.0}, ContourStyle → {Thickness[0.006], Green}]
congr11 = ContourPlot[p1[s, a], {s, -4.04, 4.04}, {a, -4.04, 4.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Thickness[0.004]}]
congr33 = ContourPlot[p3[s, a], {s, -4.04, 4.04}, {a, -4.04, 4.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Thickness[0.004]}]
congr13 = ContourPlot[-p1[s, a] + p3[s, a], {s, -4.04, 4.04}, {a, -4.04, 4.04},
  ContourShading → False, PlotPoints → 55,
  Contours → {0.0}, ContourStyle → {Black, Thickness[0.00777]}]
conX = ContourPlot[p1[s, a] - 0.202350043807531 * p3[s, a],
  {s, -4.04, 4.04}, {a, -4.04, 4.04},
  ContourShading → False, PlotPoints → 55, Contours → {0.0},
  ContourStyle → {Thickness[0.005], Red}]

```

```
BildSP2 = Show[ConSummit, deter1, congr11, congr33, congr13, conX]
```



```

N = 14 SP3 halb
stat point detHess - 0.986 SP3
node323 = {3.1507371778, 6.2862332995, 9.4247774088,
12.5633220701, 15.6988181918, 18.8434592622,
21.9820037110, 25.1296928966, 28.2743337549,
31.4189747405, 34.5666639262, 37.7052085024,
40.8498497002, 43.9853458218}
Setxx = node323

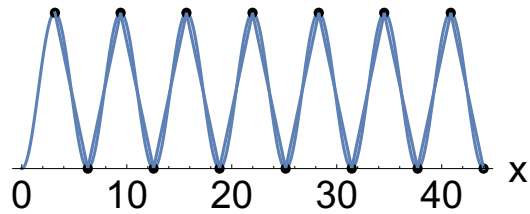
```

```
SetX = {3.1550779462792438, 6.283185715899832,
  9.411293894240668, 12.552885730501652, 15.680993091587984,
  18.836067359512928, 21.97765347442941, 25.13273428043255,
  28.287808138149902, 31.429408147742823, 34.52448998650445,
  37.70239376926342, 40.86079020006907, 43.98643016794501}
```

### Eigenvalues

```
{4.19135, 4.06085, 3.85611, 3.59843, 3.324, 3.09452, 2.41424, 0.905637,
  0.676224, -0.414132, 0.401723, -0.191167, 0.144042, -0.0606339}
```

SP3 ENERGY 14.001367005816707`



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

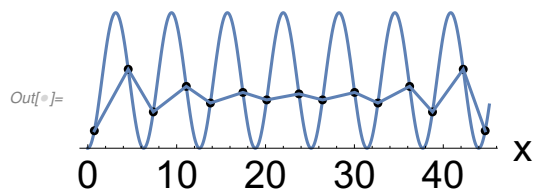
HALF N = 15 local minimum start a0

ENERGY 12.736276641075621

```
SetX = {0.73429546072, 4.545952280185356, 7.371427829572637,
  11.08271618620935, 13.797799028782224, 17.455847061193577,
  20.12953414262861, 23.761230887441755, 26.412719453262646,
  30.02221760673048, 32.647354843195934, 36.215457357184704,
  38.78735430527177, 42.24506404451186, 44.71659242330815}
```

### Eigenvalues

```
Out[ ] = {4.19613, 4.0652, 3.85241, 3.56571, 3.21511, 2.81581, 2.4532, 2.18469,
  1.75456, 1.32624, 0.963431, 0.666846, 0.442754, 0.298997, 0.24387}
```





SP2 energy = 15.49648524 detHess 15.25817044  
 would be a singular NT to SP2  
 3.8709393021 × 6.3504669656 × 8.8972255370  
 11.9474041514 × 14.4173890890 × 17.8483680499  
 20.4372348100 × 24.0259590651 × 26.7204201172  
 30.4147386642 × 33.2669450105 × 37.0801453801  
 40.3131520729 × 44.0495788087 × 47.8532364524  
 sp node155 energy = 15.9993614 detHess - 4.4789  
 3.1330422730 × 6.2774850198 × 9.4162275102  
 12.5635203470 × 15.7079629204 × 18.8524058413  
 21.9996986782 × 25.1384415161 × 28.2828846105  
 31.4187770809 × 34.5575200923 × 37.6962622010  
 40.8321546713 × 43.9765968629 × 47.1153387980  
 node228 energy = 15.49676245 detHess 18.67991  
 2.4114084361 × 6.2152955968 × 9.9513451858  
 13.1848262289 × 16.9980847980 × 19.8504746311  
 23.5448314746 × 26.2393347478 × 29.8280167816  
 32.4168452453 × 35.8476407193 × 38.3175674576  
 41.3672717219 × 43.9144074401 × 46.3937055869  
 node306 energy = 12.73710997 detHess 534.65  
 5.5414511559 × 8.0145953509 × 11.4748688670  
 14.0478219325 × 17.6167863874 × 20.2423399732  
 23.8520911705 × 26.5036403281 × 30.1352764775  
 32.8087105873 × 36.4663423087 × 39.1805631610  
 42.8907954027 × 45.7137071938 × 49.5237483061  
 node420 energy = 14.000158 detHess 3.27 E - 003  
 6.2882333245 × 9.4348734809 × 12.5714182887  
 15.7130107493 × 18.8495557500 × 21.9861005793  
 25.1276933829 × 28.2642383622 × 31.4108786901  
 34.5524711936 × 37.6991116716 × 40.8457519781  
 43.9873448246 × 47.1339853240 × 50.2705304747  
 node534 energy = 12.73686293 detHess 558.6  
 7.0022242850 × 10.8171216173 × 13.6478994168  
 17.3613545603 × 20.0782187291 × 23.7371239174  
 26.4113337498 × 30.0431549486 × 32.6945190571  
 36.3034945318 × 38.9277746508 × 42.4940957892  
 45.0638259528 × 48.5162334604 × 50.9845214353

```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

```
HALF N = 15 search SP1
```

```
node81 = {3.8709393021, 6.3504669656, 8.8972255370,  
11.9474041514, 14.4173890890, 17.8483680499,  
20.4372348100, 24.0259590651, 26.7204201172,  
30.4147386642, 33.2669450105, 37.0801453801,  
40.3131520729, 44.0495788087, 47.8532364524}
```

```
LiMin = {0.734295460722444, 4.545952280185356, 7.371427829572637,  
11.08271618620935, 13.797799028782224, 17.455847061193577,  
20.12953414262861, 23.761230887441755, 26.412719453262646,  
30.02221760673048, 32.647354843195934, 36.215457357184704,  
38.78735430527177, 42.24506404451186, 44.71659242330815}
```

```
Setxx = 0.5 * (LiMin + node81) is again SP2
```

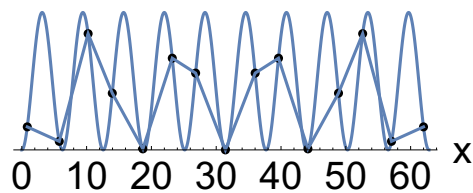
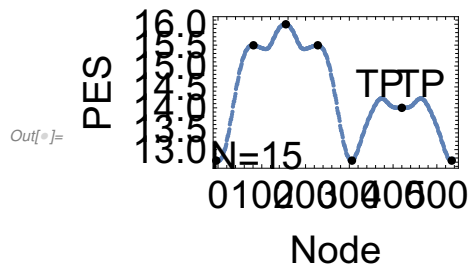
```
Setxx = 1. / 3. * (2. * LiMin + node81)
```

```
it is a ?Min
```

```
Out[8]= {0.734295, 4.54595, 7.37143, 11.0827, 13.7978, 17.4558, 20.1295,  
23.7612, 26.4127, 30.0222, 32.6474, 36.2155, 38.7874, 42.2451, 44.7166}
```

**Eigenvalues**

```
Out[9]= {4.19613, 4.0652, 3.85241, 3.56571, 3.21511, 2.81581, 2.4532, 2.18469,  
1.75456, 1.32624, 0.963431, 0.666846, 0.442754, 0.298997, 0.24387}
```

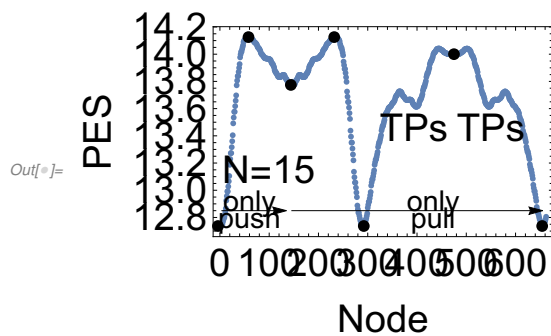


GlobMinA0

```

pull only SP node 58 energy = 14.12569821 detHess - 96.14
3.8832676111 × 6.3449898800 × 8.8684773823
11.9200131012 × 14.3692661474 × 17.7917048722
20.3428406901 × 23.8909739923 × 26.4927507803
30.0723941703 × 32.6777510539 × 36.2357546630
38.7995243042 × 42.2546883205 × 44.7221222389
iMin node144 energy = 13.77401784 detHess 32.9293159
5.4792806683 × 7.8973213892 × 11.3144230900
13.7819278734 × 17.1869960213 × 19.5962714922
22.6847788706 × 25.1339534165 × 27.5843401498
30.6712592315 × 33.0804511009 × 36.4852536936
38.9530852501 × 42.3711468354 × 44.7900225324

```



```

### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##

```

```

HALF N = 15 global SP start a0 + Pi

```

```

Setxx = Table[a0 * (i - 1) + Pi, {i, 15}]

```

```

SetX = {3.141476504544989, 6.283185307180002, 9.42489410981543,
12.5664867634046, 15.708195566038464, 18.84967207058398,
21.99126472417399, 25.132741228718352, 28.274217733262716,
31.415810386852716, 34.55728689139823, 37.69899569403209,
40.84058834762126, 43.982297150256684, 47.1240059528917}

```

```

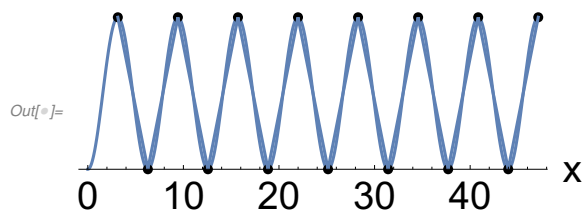
Eigenvalues

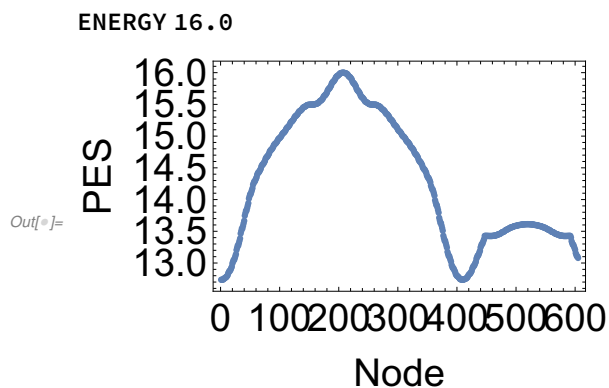
```

```

Out[ ] = {4.19828, 4.08787, 3.91397, 3.69288, 3.4502, 3.22338, 3.05966, 0.925938,
0.733751, 0.483264, -0.415069, -0.413335, 0.226414, -0.167206, 1.27411 × 10-8}

```

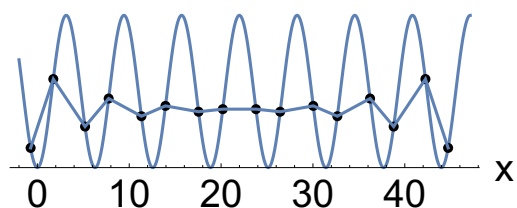




```

## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
HALF N = 16 global minimum start a0
Setxx = Table[a0 * (i - 1), {i, 16}]
ENERGY 13.61451701290423
SetX = {-0.7357862485058007, 1.7346361866005833, 5.191666734571228,
  7.761369294074385, 11.326786428162393, 13.946554658813021,
  17.54821152485848, 20.18595144599161, 23.79634512662687, 26.4340850785003,
  30.035741935011075, 32.65551031103746, 36.22092746637777,
  38.79063001204342, 42.247660694576496, 44.718083244925154}
Eigenvalues
{4.2015, 4.08629, 3.89849, 3.6444, 3.33205, 2.97145, 2.59628, 2.32038,
  2.0052, 1.57917, 1.20171, 0.879913, 0.61707, 0.419056, 0.292626, 0.244269}

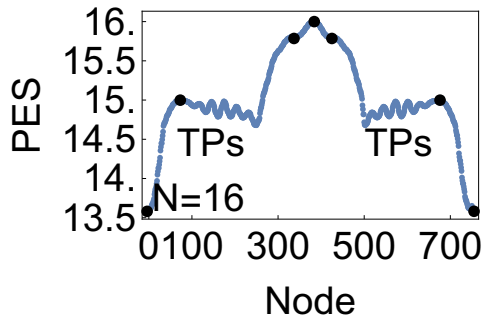
```



```

stat point
energy = 14.998762 detHess - 150.14775 SP1
node73 = {-0.7281896638 × 1.7439067326 × 5.2010569042 ×
7.7752480904 × 11.3463413927 × 13.9783252970 ×
17.5977203708 × 20.2675536339 × 23.9257358876 ×
26.6493635058 × 30.3715240734 × 33.2290601626 ×
37.0573759933 × 40.2871049651 × 44.0425864622 ×
47.8583207544}
energy = 15.804634 detHess 4.0259380
node337 = {-0.5663517810 × 2.0363294679 × 5.5325930827 ×
8.3467847331 × 12.0419865664 × 15.2365084882 ×
18.8852132512 × 22.5695677883 × 25.7072213418 ×
29.3882733274 × 32.1718818624 × 35.6414744904 ×
38.2272519697 × 41.3169572049 × 43.9482103277 ×
46.5453832286}
energy = 15.999985 detHess - 1.0152161 SP 3
node384 = {-0.0000002117 × 3.1377578385 × 6.2793506956 ×
9.4171089502 × 12.5625361416 × 15.7041288697 ×
18.8495559867 × 21.9949831687 × 25.1365757665 ×
28.2820028927 × 31.4197610837 × 34.5613538129 ×
37.6991119282 × 40.8368701285 × 43.9784626876 ×
47.1162207932}
energy = 15.804633 detHess 4.830
node425 = {0.5661163876 × 4.2466194957 × 7.0336463573 ×
10.5026492517 × 13.0906996576 × 16.1793823605 ×
18.8139140164 × 21.4128113130 × 24.5583409715 ×
27.1605392366 × 30.6601170676 × 33.4738169417 ×
37.1712135488 × 40.3648912964 × 44.0166305130 ×
47.7026963474}
energy = 14.998755 detHess - 168.6
node676 = {0.7269417110 × 4.5383041354 × 7.3647810973 ×
11.0739668840 × 13.7862237971 × 17.4375296031 ×
20.1014129126 × 23.7148647557 × 26.3399860726 ×
29.8997472176 × 32.4609995007 × 35.8872129406 ×
38.3423510811 × 41.3972797045 × 43.9239269122 ×
46.3922370214}
energy = 13.61459 detHess 844.57 Min
node747 = {0.7448716950 × 4.5556398161 × 7.3786679538 ×
11.0908453113 × 13.8075575212 × 17.4704385673 ×
20.1516338510 × 23.7969410833 × 26.4697330851 ×
30.1153171039 × 32.7971800938 × 36.4611335683 ×
39.1799616247 × 42.8947472171 × 45.7240416751 ×
49.5387600386}

```



N = 16 SP2 near top of the profil

energy = 15.804634 detHess 4.0259380

```
node337 = {-0.5663517810, 2.0363294679, 5.5325930827,
8.3467847331, 12.0419865664, 15.2365084882,
18.8852132512, 22.5695677883, 25.7072213418,
29.3882733274, 32.1718818624, 35.6414744904,
38.2272519697, 41.3169572049, 43.9482103277,
46.5453832286}
```

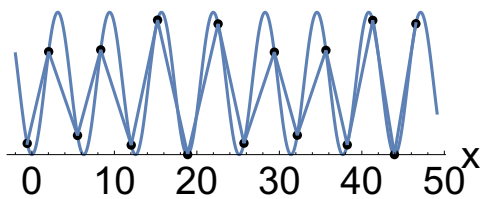
Setxx = node337

```
SetX = {-0.5691509801983105, 2.0335246096635413, 5.531038147645141,
8.345343445356487, 12.041339880028517, 15.23609671511133,
18.885403204993068, 22.570549301363496, 25.70817282943925,
29.389993293537547, 32.173612907107646, 35.64447512196629,
38.23012236477882, 41.322174575802904, 43.95114415800876, 46.54896578676459}
```

SP2 ENERGY 15.804635032127027

Eigenvalues

```
{4.207960178955515, 4.101965749220275, 3.933965865571099, 3.719476593183895,
3.458788708226801, 3.228899694826447, 2.940514443974855,
2.3632199332766772, 1.2882709317530607, 1.0350896582128755,
0.7311416787429645, 0.463150066954638, -0.28134263699175577,
0.27435343413014124, 0.1627801560219897, -0.03983656979868755}
```



sp2Half

energy = 15.999985 detHess - 1.0152161 SP 3

```
node384 = {-0.0000002117, 3.1377578385, 6.2793506956,
9.4171089502, 12.5625361416, 15.7041288697,
18.8495559867, 21.9949831687, 25.1365757665,
28.2820028927, 31.4197610837, 34.5613538129,
37.6991119282, 40.8368701285, 43.9784626876,
47.1162207932}
```

Setxx = node384

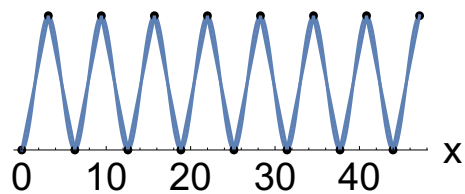
```
SetX = {-4.2110821173319205`*^-13, 3.1415926535891576, 6.283185307179372,
  9.424777960769372, 12.566370614359379, 15.707963267949593,
  18.849555921539178, 21.99114857512918, 25.132741228718555,
  28.27433388230814, 31.415926535897725, 34.557519189487095,
  37.6991118430771, 40.84070449666668, 43.9822971502569, 47.12388980384691}
```

SP3 ENERGY 16.0

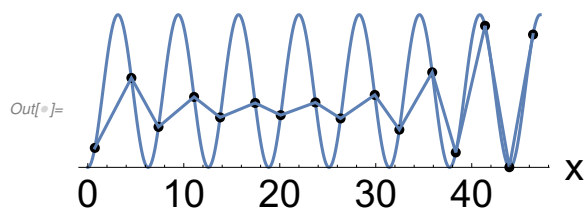
Eigenvalues

```
{4.201762717692934, 4.101002989615459, 3.9404553240747853, 3.732050807568877,
  3.494868935816723, 3.2592801267497657, 3.073424862287728,
  2.414213562373095, 0.9265751377122755, 0.7407198732502369,
  0.5051310641832818, -0.41421356237310114, 0.2679491924311259,
  -0.2017627176929322, -0.1010029896154565, 0.05954467592521784}
```

ENERGY 16.0



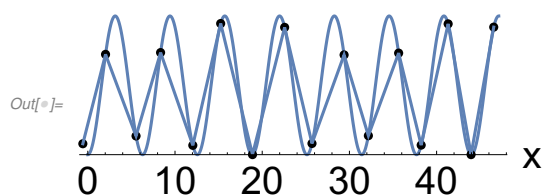
```
start energy 13.614517
-0.735786 × 1.734640 × 5.191670 × 7.76137
11.326800 × 13.946600 × 17.548200 × 20.186
23.796300 × 26.434100 × 30.035700 × 32.6555
36.220900 × 38.790600 × 42.247700 × 44.7181
stat SP1 node213 energy = 14.99720288 detHess - 186.22
node213 = {0.7304637441, 4.5398692076, 7.3647170099,
  11.0728411956, 13.7845466603, 17.4353208019,
  20.0989233122, 23.7119084526, 26.3367147450,
  29.8955902725, 32.4563363152, 35.8802916277,
  38.3354451891, 41.3854468527, 43.9178484377,
  46.3864435934}
node213
```



```

node309 energy = 15.80356809 detHess 4.69181886 SP2
node309 = {-0.5690274559, 2.0337838518, 5.5313490162,
8.3459646389, 12.0420097945, 15.2374268078,
18.8862399941, 22.5717606878, 25.7087772000,
29.3905292520, 32.1738766450, 35.6446898641,
38.2302198992, 41.3222706657, 43.9511853016,
46.5490247696}
SetX = node309

```



```

node404 energy = 15.001072742 detHess - 150.628
-0.7317996732 × 1.7414182906 × 5.1999505403
7.7748398977 × 11.3464341172 × 13.9787857397
17.5984561909 × 20.2686307621 × 23.9271526254
26.6514598295 × 30.3742462303 × 33.2336139519
37.0624935033 × 40.2967283732 × 44.0483404523
47.8657827683
node605 energy = 13.62913289 detHess 845.86
0.6685933132 × 4.4513833234 × 7.2890576844
10.9927013374 × 13.7175458283 × 17.3769421507
20.0624571237 × 23.7059226120 × 26.3810266994
30.0259922866 × 32.7081109362 × 36.3733539876
39.0886699745 × 42.8090540050 × 45.6287320444
49.4671993865

```



\*\*\* \*\* \*\* \*\* \*\*

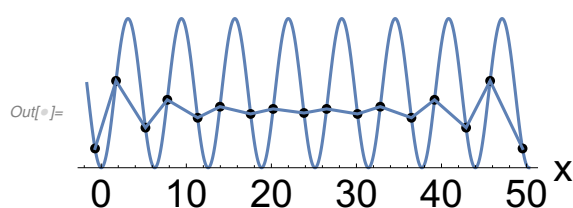
N = 17 HALF global minimum start a0

ENERGY 14.491533125784821

SetX = {-0.7348704086803581, 1.7362311830352526,  
5.193679552870021, 7.764729700912525, 11.33179947897368,  
13.954862406991229, 17.56135374413623, 20.207509744847997,  
23.83110026450109, 26.490694986328425, 30.127724208458226,  
32.80441793830392, 36.46454027294931, 39.180655721055274,  
42.892791027380326, 45.71852797315353, 49.53061181462928}

Eigenvalues

Out[\*]= {4.20594, 4.1038, 3.93692, 3.7103, 3.43049, 3.1052, 2.74893, 2.43578, 2.18996,  
1.8179, 1.43324, 1.09669, 0.809068, 0.574552, 0.398377, 0.286368, 0.243595}



first peak is mirror for the asymmetry of min

min ? node115 energy = 15.9585922 detHess 2.06181

0.3675887059 × 3.8744291228 × 6.7122889260  
9.9662045846 × 12.7047611467 × 15.5812669227  
18.5841303618 × 21.3246738519 × 24.6834362879  
27.6078591588 × 31.1505009758 × 34.4308228434  
37.8375023749 × 41.3821311200 × 44.4114007688  
47.8567262727 × 50.6330711631

sp node141 energy = 15.999982 detHess - 0.994382

-0.0016298691 × 3.1367032030 × 6.2799257061  
9.4198886140 × 12.5647408492 × 15.7079633199  
18.8511857387 × 21.9960379738 × 25.1360008298  
28.2792232810 × 31.4175563530 × 34.5575192414  
37.6974820779 × 40.8358151499 × 43.9790375492  
47.1190003532 × 50.2638525884

node167 energy = 15.958652 detHess 2.57578

-0.3865967068 × 2.3847119628 × 5.8426777419  
8.8742448902 × 12.4289536495 × 15.8466775194  
19.1261315584 × 22.6786486294 × 25.5965585783  
28.9618339369 × 31.6925021732 × 34.6962334418  
37.5616948787 × 40.2901714267 × 43.5417895853  
46.3670091135 × 49.8788857509

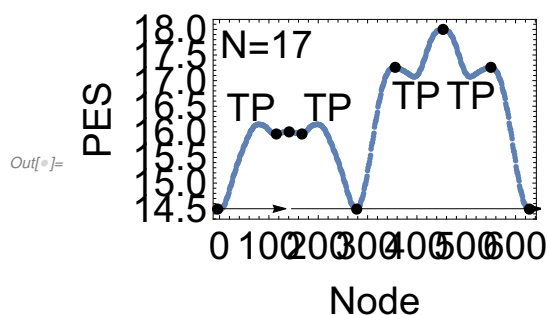
node278 energy = 14.492389 detHess 1483.428

0.7270470979 × 4.5408173311 × 7.3692699098  
11.0825317974 × 13.7995721074 × 17.4601664473  
20.1371699356 × 23.7743445477 × 26.4339912899  
30.0575298549 × 32.7035405500 × 36.3097223688  
38.9323133361 × 42.4984583333 × 45.0683817528

```

48.5231144813 × 50.9925295553
node356 energy = 17.25918 detHess 40.388
3.8872777878 × 6.3543654955 × 8.8925732997
11.9382154121 × 14.3962044156 × 17.8208303965
20.3888142079 × 23.9563007381 × 26.6005430160
30.2394860453 × 32.9551848222 × 36.6703863180
39.5289456444 × 43.3541419484 × 46.5916851437
50.3366626466 × 54.1527602467
SP2 ? node453 energy = 17.999798 detHess 0.9985
3.1455738787 × 6.2871662905 × 9.4327396751
12.5703514294 × 15.7119439884 × 18.8495558374
21.9871676023 × 25.1287603295 × 28.2663721680
31.4119456367 × 34.5535382167 × 37.6991117590
40.8446852171 × 43.9862779653 × 47.1318515181
50.2694634407 × 53.4110563362
node550 energy = 17.259429 detHess 50.469
2.3983892480 × 6.2137687193 × 9.9597873384
13.1959568507 × 17.0209367381 × 19.8789692369
23.5939985411 × 26.3095415186 × 29.9484669284
32.5927268261 × 36.1603691564 × 38.7285251591
42.1536779675 × 44.6118833864 × 47.6588991803
50.1960658684 × 52.6638717032
node628 energy = 14.4927611 detHess 1410.808
5.5481603628 × 8.0192954514 × 11.4767973016
14.0478696546 × 17.6149576541 × 20.2380299066
23.8445274322 × 26.4906864204 × 30.1142780026
32.7738717280 × 36.4108980472 × 39.0875858289
42.7476988836 × 45.4637961913 × 49.1759091452
52.0015926023 × 55.8136428208

```



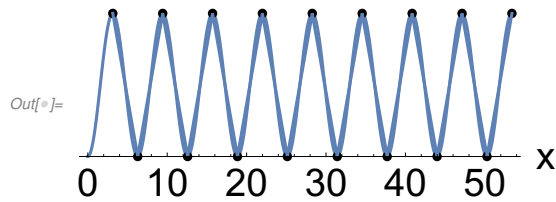
```

SP_4 node453 energy = 17.999798 detHess 0.9985
node453 = {3.1455738787, 6.2871662905, 9.4327396751,
12.5703514294, 15.7119439884, 18.8495558374,
21.9871676023, 25.1287603295, 28.2663721680,
31.4119456367, 34.5535382167, 37.6991117590,
40.8446852171, 43.9862779653, 47.1318515181,
50.2694634407, 53.4110563362}

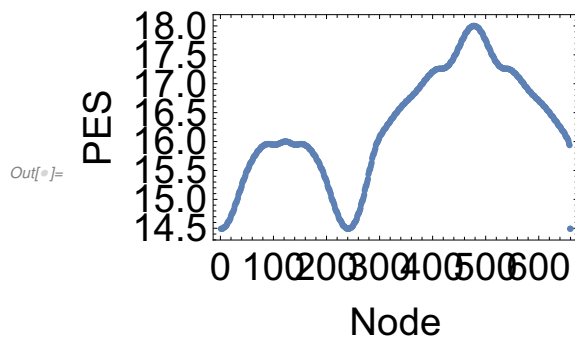
```

Eigenvalues

```
{4.206499654410857, 4.11956504614404, 3.9807074751017946, 3.7995022831767526,
 3.590616377063207, 3.3753814903559087, 3.183130035643948, 3.0484499932541653,
 0.9410448826557194, 0.7841839991497119, 0.5715818617028661,
 -0.41457020921930154, -0.41385228711746, 0.3426107874379314,
 -0.18539765439553957, 0.12638757703646064, -0.05584131240104284}
```



is globSP N = 17 NT to 11 .. 1 .. 11



N = 17 HALF SP2 But where is the corresponding SP1 ?

node356 energy = 17.25918 detHess 40.388

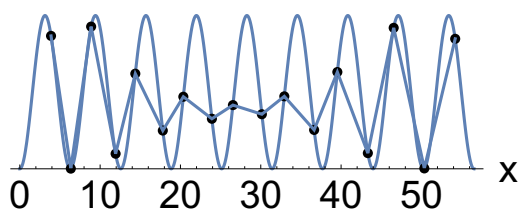
```
node356 = {3.8872777878, 6.3543654955, 8.8925732997,
11.9382154121, 14.3962044156, 17.8208303965,
20.3888142079, 23.9563007381, 26.6005430160,
30.2394860453, 32.9551848222, 36.6703863180,
39.5289456444, 43.3541419484, 46.5916851437,
50.3366626466, 54.1527602467}
```

Setxx = node356

```
SetX = {3.8876349201870943, 6.350489974140382, 8.880598892456504,
11.928423725578025, 14.380701166647595, 17.80347042327239,
20.36077083795343, 23.916296805428633, 26.5339512089223, 30.137260277857692,
32.93217407223493, 36.643877637565964, 39.53563384574823,
43.33118385137668, 46.54939361656266, 50.364602516954925, 54.2076782517958}
```

Eigenvalues

```
{4.203347689365806, 4.114916588659489, 3.9660676516749795, 3.7717622657805157,
3.5572894391196144, 3.322382435807474, 3.0486417466637175,
2.5844424625304683, 1.815411758166333, 1.292212622973795, 0.9442801631658799,
0.6667973317159244, 0.4518127464458086, 0.292437182792852,
0.2281978409459544, -0.20593709469797705, -0.18011815713344959}
```



SPindex2Half

seach SP\_1 beteen min und SP\_2

MIN node 278 energy = 14.492389 detHess 1483.428

node278 = {0.7270470979, 4.5408173311, 7.3692699098,  
11.0825317974, 13.7995721074, 17.4601664473,  
20.1371699356, 23.7743445477, 26.4339912899,  
30.0575298549, 32.7035405500, 36.3097223688,  
38.9323133361, 42.4984583333, 45.0683817528,  
48.5231144813, 50.9925295553}

nodexx = 1. / 7. \* ( 2.0 \* node356 + 5.0 \* node278)

Setxx = nodexx

Out[\*]= {0.734871, 4.54695, 7.37269, 11.0848, 13.8009, 17.4611, 20.1378, 23.7748, 26.4344,  
30.058, 32.7041, 36.3106, 38.9337, 42.5008, 45.0718, 48.5293, 51.0004}

Eigenvalues

Out[\*]= {4.20594, 4.1038, 3.93692, 3.7103, 3.43049, 3.1052, 2.74893, 2.43578, 2.18996,  
1.8179, 1.43324, 1.09669, 0.809068, 0.574552, 0.398377, 0.286368, 0.243595}

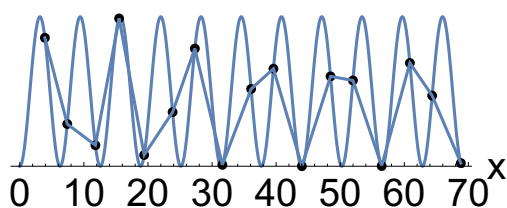
nodexx = 1. / 2. \* ( node356 + node278)

SetX = {3.8783728217211744, 6.348058367741061, 8.882571356011908,  
11.933111684752657, 14.391877160467816, 17.818379150727292,  
20.386977092381557, 23.955018337029458, 26.59932356693661,  
30.23820363981408, 32.95334769986086, 36.667935065512204, 39.52461837903441,  
43.34903820701192, 46.58168316726568, 50.330355488740445, 54.143855217548335}

Eigenvalues

Out[\*]= {4.21041, 4.11934, 3.96992, 3.7758, 3.55957, 3.33032, 3.04869, 2.61741, 1.79321,  
1.29931, 0.941302, 0.664458, 0.447978, 0.288453, 0.228219, -0.210241, -0.210061}

ENERGY 17.259103 is another SP2 with same energy



for barrier now emerge two copeting peaks !

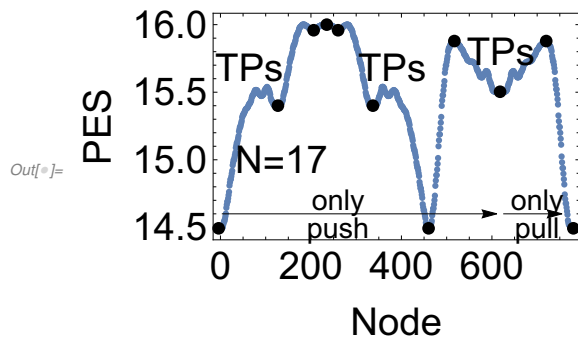
start gMin

-0.73487 × 1.73623 × 5.19368 × 7.76473

11.3318 × 13.9549 × 17.5614 × 20.2075  
 23.8311 × 26.4907 × 30.1277 × 32.8044  
 36.4645 × 39.1807 × 42.8928 × 45.7185 × 49.5306

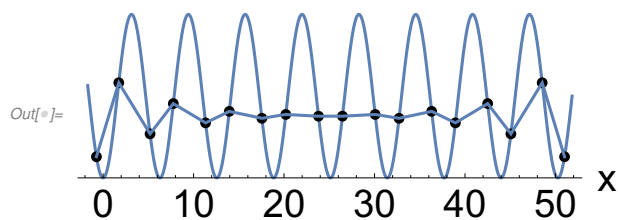
SP node127 energy = 15.4005363 detHess - 2.225  
 0.6824676942 × 4.4542773986 × 7.2592133727  
 10.8924277152 × 13.5309569506 × 16.9912994849  
 19.4926749481 × 22.5937447018 × 25.1280312109  
 27.6576077197 × 30.7655517744 × 33.2680111242  
 36.7311690972 × 39.3706060662 × 43.0049772873  
 45.8103470156 × 49.5828091415  
 iMin ? node206 energy = 15.95813138 detHess 2.310272  
 -0.3798732040 × 2.3940120595 × 5.8477638373  
 8.8797230328 × 12.4301472884 × 15.8447691388  
 19.1230114587 × 22.6713139625 × 25.5906948501  
 28.9521892537 × 31.6865596828 × 34.6882717036  
 37.5596034542 × 40.2918789083 × 43.5458400164  
 46.3770697398 × 49.8876080571  
 SP node 235 energy = 15.99949302 detHess - 0.9908907  
 -0.0000001001 × 3.1392527593 × 6.2808455109  
 9.4200984683 × 12.5640309011 × 15.7056236228  
 18.8495559875 × 21.9934884183 × 25.1350810080  
 28.2790133748 × 31.4182662662 × 34.5598588858  
 37.6991118112 × 40.8383647047 × 43.9799573881  
 47.1192103114 × 50.2631427101  
 node262 energy = 15.958270 detHess 2.4060112  
 0.3836569261 × 3.8929170398 × 6.7195699528  
 9.9688885565 × 12.7005498285 × 15.5659880485  
 18.5729250035 × 21.3067457468 × 24.6727769278  
 27.5948919902 × 31.1453660093 × 34.4285684144  
 37.8403645195 × 41.3929440497 × 44.4209283895  
 47.8736134071 × 50.6448619272  
 node337 energy = 15.40048451 detHess - 1.540279588  
 -0.6820914204 × 1.8284535172 × 5.3059880791  
 7.9545897366 × 11.5981346673 × 14.4177923858  
 18.1983325096 × 21.3727127423 × 25.1268543834  
 28.8751092132 × 32.0580818309 × 35.8399772546  
 38.6631549483 × 42.3078363102 × 44.9578860276  
 48.4359679491 × 50.9473311559  
 gMin node 462 energy = 14.49359819 detHess 1477.1247  
 0.7475362609 × 4.5568273643 × 7.3781937951  
 11.0884923626 × 13.8031047093 × 17.4624352598  
 20.1385868147 × 23.7753044236 × 26.4346969611  
 30.0581689980 × 32.7042481004 × 36.3106957854  
 38.9337287028 × 42.5007835016 × 45.0718213519  
 48.5292659673 × 51.0003613273  
 SP node517 energy = 15.878581 detHess - 234.879  
 3.9082414261 × 6.3638343681 × 8.8999889722  
 11.9371739767 × 14.3858635521 × 17.8037871900

20.3564007178  $\times$  23.9069700447  $\times$  26.5164724224  
 30.1085290827  $\times$  32.7350751295  $\times$  36.3301246287  
 38.9454685688  $\times$  42.5086420281  $\times$  45.0765299851  
 48.5329945331  $\times$  51.0025027123  
 flat iMin node608 energy15.50345 detHess 27.413  
 5.4899186634  $\times$  7.9170063185  $\times$  11.3421085755  
 13.8266553785  $\times$  17.2633795701  $\times$  19.7002220320  
 22.8887843540  $\times$  25.2954915776  $\times$  27.8642316213  
 30.8316747766  $\times$  33.2475425214  $\times$  36.6295892015  
 39.1346646685  $\times$  42.6306086644  $\times$  45.1504609038  
 48.5903457745  $\times$  51.0356691634



-----  
 N = 18 global minimum start a0  
 ENERGY 15.3693023888189  
 SetX = {-0.7354348524812376, 1.7352481174085652, 5.192439272562506,  
 7.762658904505984, 11.328711501387344, 13.949743087121709,  
 17.553262117757264, 20.194221056598035, 23.80972112686948,  
 26.455761153557823, 30.071261234301513, 32.71222018161424,  
 36.31573925187848, 38.93677082386414, 42.50282339725018,  
 45.07304300553948, 48.5302342593662, 51.00091719829504}  
 Eigenvalues

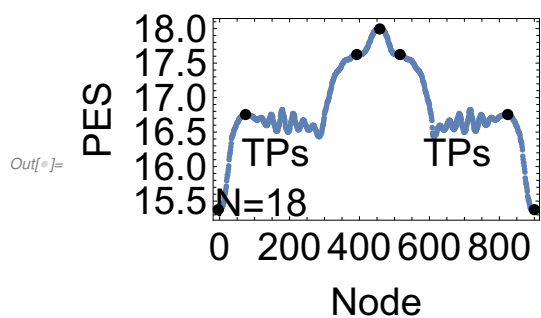
Out[ $\ast$ ]= {4.20966, 4.11849, 3.96921, 3.76587, 3.51382,  
 3.21933, 2.89098, 2.56183, 2.31464, 2.03236, 1.65653, 1.31163,  
 1.00875, 0.749934, 0.539371, 0.381631, 0.281749, 0.243634}



```

SP node74 energy = 16.754597 detHess - 384.10
-0.7310440552 × 1.7399399798 × 5.1966533056
7.7683489437 × 11.3363803454 × 13.9619261977
17.5721566459 × 20.2251201401 × 23.8590863032
26.5368751079 × 30.2008078445 × 32.9273298471
36.6520886032 × 39.5109091243 × 43.3408292044
46.5723770537 × 50.3279011901 × 54.1458035356
iMin ? exists not !
node392 4.7 energy = 17.624344 detHess 10.71495
0.6436266773 × 1.9012318981 × 5.3919915836
8.1049287313 × 11.7865435506 × 14.7650019040
18.5527613912 × 22.0480644868 × 25.4864823949
29.2713100520 × 32.2163043513 × 35.8789179168
38.5724702002 × 42.0325126640 × 44.5635156554
47.6435614105 × 50.2270120406 × 52.7720017423
node458 energy = 17.99506688 detHess - 4.826
0.0140598456 × 3.1798294114 × 6.3077280505
9.4475981442 × 12.5911569433 × 15.7433291961
18.8798478775 × 22.0368106595 × 25.1498282642
28.2710869502 × 31.3977194565 × 34.5018510625
37.6406793639 × 40.7217715384 × 43.9040706437
47.0127742905 × 50.1940899882 × 53.3260870131
node516 energy = 17.623555 detHess 14.43616
0.6346081895 × 4.3738218925 × 7.1698040403
10.7407252875 × 13.3439451610 × 16.6487180992
19.1454879766 × 21.9338893701 × 24.7795186852
27.2792248091 × 30.6177492849 × 33.2401887822
36.8306774012 × 39.6578475328 × 43.4107081903
46.6225997341 × 50.3150485599 × 54.0570431950
SP node824 energy = 16.75590857 detHess - 444.05
0.7343508130 × 4.5458287889 × 7.3711458749
11.0821448246 × 13.7968886635 × 17.4542943295
20.1270666990 × 23.7571382635 × 26.4061996438
30.0113808280 × 32.6303498454 × 36.1864872202
38.7443160916 × 42.1671719957 × 44.6197279962
47.6674167619 × 50.1979476374 × 52.6609950184
gMin node895 energy = 15.37506496 detHess 2311.64
0.7228108646 × 4.5380312720 × 7.3684135155
11.0832057038 × 13.8018350681 × 17.4647655803
20.1449453869 × 23.7874398295 × 26.4552507058
30.0923964220 × 32.7599569882 × 36.4019161640
39.0810710947 × 42.7424492252 × 45.4580927605
49.1692271207 × 51.9908589300 × 55.8005670001

```



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

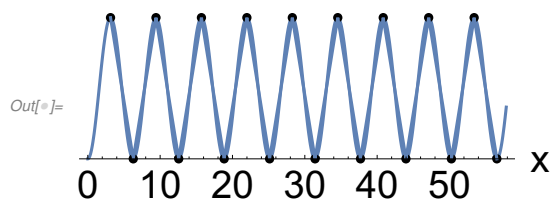
```
N = 18 global SP start a0 + Pi
```

```
Setxx = Table[a0 * (i - 1) + Pi, {i, 18}]
```

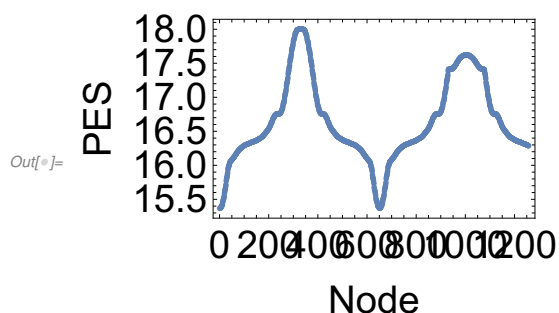
```
SetX = {3.1414665916655, 6.2831853071801, 9.42490402269515,
12.566496676284105, 15.70821539179700, 18.84968198346324,
21.991274637052964, 25.13274122871796, 28.27420782038258,
31.41580047397307, 34.557267065639685, 37.69898578115297,
40.840578434742696, 43.98229715025735, 47.12401586577225,
50.265608519361486, 53.40732723487453, 56.54879382654089}
```

```
Eigenvalues
```

```
Out[ ] = {4.20893, 4.12887, 4., 3.82956, 3.62871, 3.41421, 3.21157,
3.05859, 2.41421, 0.941409, 0.788426, 0.585786, -0.414214,
0.371288, -0.208933, 0.170438, -0.12887, 1.58916 × 10-8}
```



```
ENERGY 18.0
```





```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

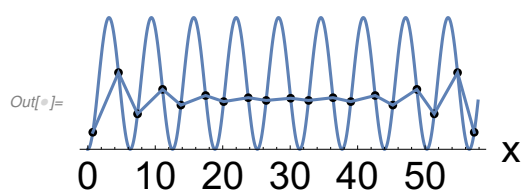
```
N = 19 Half global minimum start a0
```

```
ENERGY 16.24660801532827
```

```
SetX = {0.73508762952066, 4.54733259675176, 7.373168521021862,
  11.085623538540702, 13.802130392201244, 17.463035585792987,
  20.140871465305914, 23.77990614160327, 26.442600450149186,
  30.071443373336162, 32.72578585459652, 36.346276874844115, 38.9904275272662,
  42.595776982926786, 45.218057204545076, 48.78473585763304,
  51.355466047082516, 54.812815453260036, 57.283755754191745}
```

```
Eigenvalues
```

```
Out[ ] = {4.21281, 4.13094, 3.99665, 3.81324, 3.58511, 3.31748,
  3.01662, 2.69692, 2.42136, 2.19424, 1.86673, 1.51935, 1.20764,
  0.933299, 0.699146, 0.509076, 0.367061, 0.277466, 0.243277}
```



```
SP1 node58 energy = 17.633329 detHess - 668.36
```

```
3.8696742914 × 6.3374477523 × 8.8594570336
```

```
11.9171531550 × 14.3702860237 × 17.7963694717
```

```
20.3534486153 × 23.9082905457 × 26.5225129677
```

```
30.1203951347 × 32.7559240776 × 36.3649370000
```

```
39.0018144104 × 42.6029694201 × 45.2223986108
```

```
48.7876447500 × 51.3572084308 × 54.8141959424
```

```
57.2845484103
```

```
iMin node178 energy = 17.2382439 detHess 140.193
```

```
5.5330439820 × 7.9798248534 × 11.4186979112
```

```
13.9457601713 × 17.4545600139 × 19.9787729925
```

```
23.4070638390 × 25.8473248002 × 28.9428886791
```

```
31.4186000004 × 33.8969847830 × 36.9889085071
```

```
39.4288442715 × 42.8561762591 × 45.3807579175
```

```
48.8905265199 × 51.4194106383 × 54.8626562633
```

```
57.3125318172
```

```
Barrier19 = 17.633568 - 16.248263592
```

```
1.3853
```

```
barriere of the former cape becomes higher than the pre - SPs ..
```

```
Barrier19 = 16.248263592 - 17.9993156
```

```
-1.7511
```

```
SP node123 energy = 17.633568 detHess - 744.57
```

```
5.5472913462 × 8.0176339433 × 11.4746153680
```

```
14.0441594687 × 17.6093814940 × 20.2287628808
```

```
23.8298470971 × 26.4666029871 × 30.0754209484
```

```
32.7106388362 × 36.3079869922 × 38.9214326905
```

```
42.4747727648 × 45.0301138374 × 48.4517897163
```

```
50.9028201771 × 53.9489085618 × 56.4792892532
```

58.9403470773

gMin node178 energy = 16.248263592 detHess 3773.86

5.5480968584 × 8.0190367438 × 11.4763859381  
 14.0471153050 × 17.6137927654 × 20.2360708222  
 23.8414170557 × 26.4855621113 × 30.1060444341  
 32.7603722108 × 36.3891918665 × 39.0518472059  
 42.6908213149 × 45.3685524191 × 49.0293040912  
 51.7455199170 × 55.4576199834 × 58.2826090383  
 62.0943194481

SP1 node322 energy = 17.17920680 detHess - 80.441

5.5798807521 × 8.0747317774 × 11.5453162740  
 14.1632414164 × 17.7808266390 × 20.5218221676  
 24.2576740396 × 27.2259393430 × 31.0608279237  
 34.5480336775 × 38.0447248011 × 41.8801893779  
 44.8535106055 × 48.5919426754 × 51.3356482126  
 54.9566338252 × 57.5778449473 × 61.0559311667  
 63.5549819729

415 energy = 17.85195888 detHess 5.44

5.7828267068 × 8.4446791512 × 11.9370840012  
 14.8409206792 × 18.5071759373 × 21.8377013085  
 25.3210724751 × 28.9916635513 × 32.0048798742  
 35.5735872017 × 38.2922509574 × 41.5698814085  
 44.1812557946 × 46.9902788060 × 49.9325156350  
 52.5479041261 × 55.9205940393 × 58.7056967695  
 62.3238302683

node466 energy = 17.9993156 detHess - 1.005194

6.2805268161 × 9.4194609817 × 12.5637121016  
 15.7053047117 × 18.8495558751 × 21.9938069919  
 25.1353996951 × 28.2796508615 × 31.4185850738  
 34.5601778207 × 37.6991119396 × 40.8380461549  
 43.9796387089 × 47.1185728247 × 50.2628238946  
 53.4044164049 × 56.5486676182 × 59.6929186850  
 62.8345114881

node512 energy = 17.8519775 detHess 5.393259

6.7809230033 × 10.3999546120 × 13.1911852144  
 16.5673627270 × 19.1860896289 × 22.1350337623  
 24.9405886695 × 27.5551712985 × 30.8285087941  
 33.5476328228 × 37.1135282535 × 40.1267378502  
 43.7947842355 × 47.2764146355 × 50.6061109016  
 54.2698866624 × 57.1739884966 × 60.6634476756  
 63.3262235789

sp node 602 energy17 .1790903 detHess - 83.957

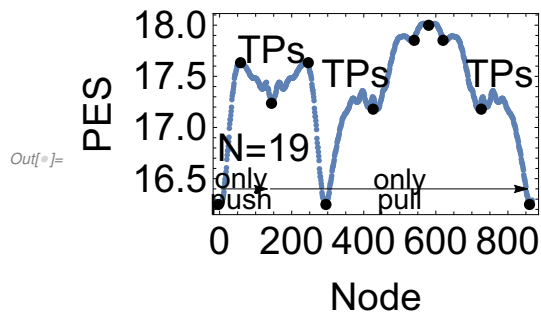
6.9860182794 × 10.7739928089 × 13.5864162348  
 17.2509715579 × 19.9159129437 × 23.4562999348  
 26.0022621673 × 29.3122443375 × 31.7608819324  
 34.5476742288 × 37.3443113269 × 39.7935451120  
 43.1087852170 × 45.6574365153 × 49.2006490160  
 51.8691532990 × 55.5371172638 × 58.3574257518  
 62.1495547152

gMin node746 energy = 16.247498651 detHess 3827.9

7.0182668709  $\times$  10.8305071888  $\times$  13.6563401741  
 17.3687859967  $\times$  20.0852814591  $\times$  23.7461639565  
 26.4239668506  $\times$  30.0629437337  $\times$  32.7255483469  
 36.3542403285  $\times$  39.0083449513  $\times$  42.6284365009  
 45.2719664581  $\times$  48.8762397882  $\times$  51.4969487633  
 55.0606356248  $\times$  57.6277454869  $\times$  61.0763780855  
 63.5420153747

sp node 801 energy = 17.6335016 detHess - 648.970

7.0190725739  $\times$  10.8319103253  $\times$  13.6581111538  
 17.3717425289  $\times$  20.0896937028  $\times$  23.7534736192  
 26.4355391594  $\times$  30.0819075569  $\times$  32.7561769919  
 36.4039882329  $\times$  39.0895571678  $\times$  42.7589068984  
 45.4879976257  $\times$  49.2149703699  $\times$  52.0742652017  
 55.9053746752  $\times$  59.1366505771  $\times$  62.8936877737  
 66.7125202753



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

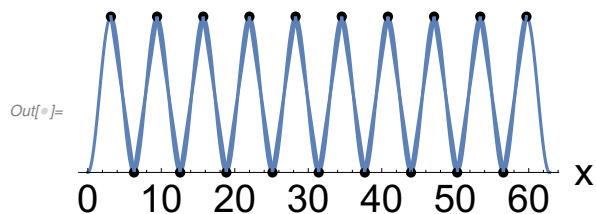
N = 19 Half global SP start  $a_0 + \pi$

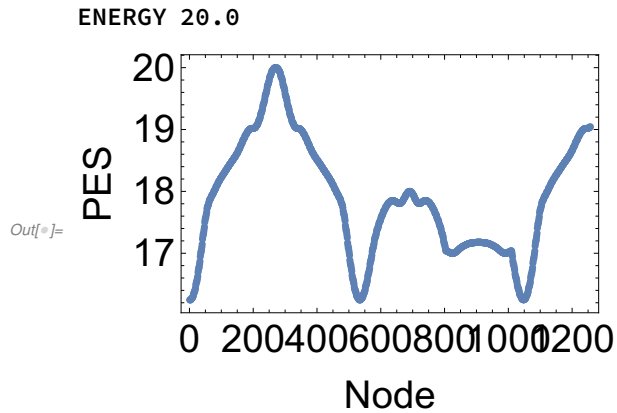
Setxx = Table[ $a_0 * (i - 1) + \pi$ , {i, 19}]

SetX = {3.1415926535902057, 6.283185307179793, 9.424777960769589,  
 12.566370614359176, 15.707963267948763, 18.849555921538553,  
 21.99114857512814, 25.132741228718135, 28.274333882307925,  
 31.41592653589793, 34.557519189487934, 37.69911184307773,  
 40.84070449666773, 43.98229715025731, 47.123889803847106,  
 50.26548245743669, 53.40707511102628, 56.54866776461607, 59.69026041820565}

Eigenvalues

Out[ ] = {4.2123, 4.14214, 4.02902, 3.87895, 3.70093, 3.5078,  
 3.31736, 3.15282, 3.04013, 0.951979, 0.82174, 0.639786, 0.436479,  
 -0.414362, -0.414064, 0.235383, -0.197409, -0.0948025, 0.0538074}





```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

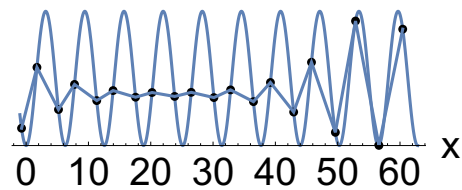
```
N = 20 HALF
```

```
SetX = {-0.73480494082218, 1.73634527078311, 5.193823523786, 7.764970208731918,
 11.33215799167777, 13.955457322206387, 17.56229283553398,
 20.209055338370423, 23.83357757977387, 26.494765695658028,
 30.134240006577834, 32.8152162663108, 36.48152128497891,
 39.20955766691434, 42.93577350990813, 45.79630110117102,
 49.627399210943445, 52.86284039529973, 56.61604510294878, 60.43657618161917}
```

Eigenvalues

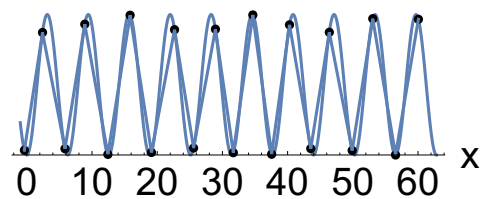
```
{4.217, 4.14678, 4.03079, 3.87349, 3.68323, 3.47064, 3.23422,
 2.95371, 2.61948, 2.28841, 1.89522, 1.51689, 1.19791, 0.926298,
 0.698384, 0.512205, 0.36835, 0.273046, 0.237891, -0.205812}
```

SP1 half ENERGY 18.50996631625231



sp1Half

SP\_3 ?



```
node160 = {0.1886164126, 3.6164995775, 6.6859175379,
10.2460594212, 13.1729723176, 16.7687544490,
19.5905850340, 23.1862536555, 25.9504583492,
29.5430401061, 32.2796953101, 35.8754371627,
38.6017729323, 42.2118775689, 44.9406311092,
48.5864101387, 51.3368355507, 55.0639008929,
57.8934546768, 61.7963674821}
```

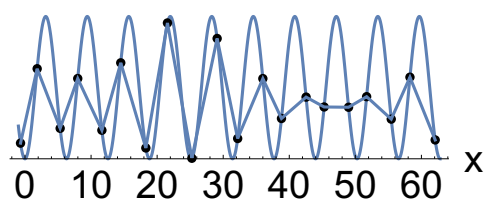
Setxx = node160 it is Shoulder 1/2 index

```
SetX = {-0.6762311966608, 1.83996278435887, 5.32096731784718,
7.982468738647075, 11.637374372694168, 14.493385611523646,
18.29049404182035, 21.561484842736235, 25.257335845025626,
29.0822348011385, 32.1902897061444, 36.0006766152135, 38.821541375356574,
42.54487932498386, 45.27796057927473, 48.97395176491473,
51.709006405199396, 55.43618381830806, 58.26668794346244, 62.08647377571958}
```

### Eigenvalues

```
{4.2208, 4.14563, 4.02951, 3.86811, 3.66951, 3.45536, 3.15169,
3.01049, 2.56122, 2.33788, 2.00658, 1.40567, 1.30515, 0.946978,
0.734965, 0.55628, 0.382622, 0.283146, 0.234647,  $-6.79019 \times 10^{-7}$ }
```

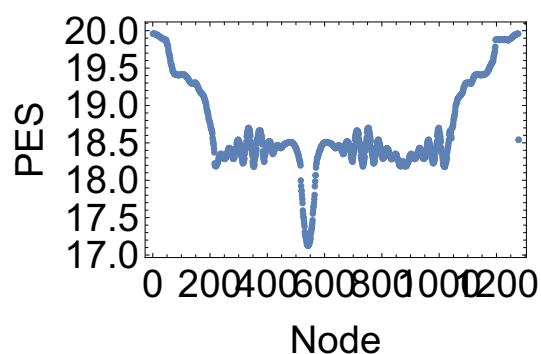
SP 1/2 ENERGY 18.05939179365861



iMin 'OBEN' energy = 19.9595 detHess 3.396

? BBP point crossed

```
node101 = {-0.3683074981 × 2.4107769419 × 5.8573386425 ×
8.8908083649 × 12.4332324319 × 15.8429112975 ×
19.1180513499 × 22.6584724753 × 25.5800074197 ×
28.9340446256 × 31.6751935157 × 34.6727145053 ×
37.5552947830 × 40.2945532578 × 43.5532139352 ×
46.3958373112 × 49.9038778259 × 53.0581427919 ×
56.5543024198 × 60.0560966732}
```



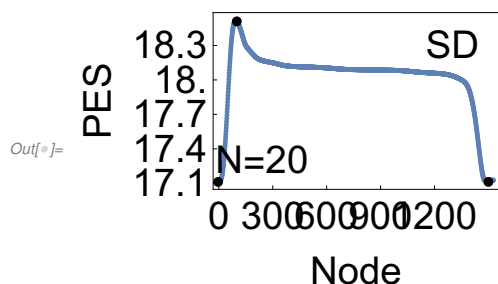
```

node106
node484 SP left energy = 18.50996
node549 gMIN energy = 17.12431
node615 SP rechts energy = 18.50996
node1007 is OBEN energy = 19.41448
node1152 node1254
node483 = {0.7380137783, 4.5493452133, 7.3739388627,
11.0855076839, 13.8011177873, 17.4607927515,
20.1369900511, 23.7733081965, 26.4318805282,
30.0537804521, 32.6973689821, 36.2993859469,
38.9159998073, 42.4706390404, 45.0270264283,
48.4482024466, 50.8996020845, 53.9434702437,
56.4762976711, 58.9368181607}
node548 = {0.7242472112, 4.5390357949, 7.3688124513,
11.0831851698, 13.8013932674, 17.4637570319,
20.1431840744, 23.7844452918, 26.4503577690,
30.0843910792, 32.7469109868, 36.3808135695,
39.0464247814, 42.6871673448, 45.3656659161,
49.0266513009, 51.7422329682, 55.4533955863,
58.2755053181, 62.0854653005}
node614 = { 3.8928455568, 6.3540178145, 8.8859633636,
11.9310278131, 14.3826388036, 17.8042725578,
20.3608395880, 23.9156362624, 26.5323323805,
30.1344086554, 32.7780349745, 36.3999648889,
39.0585651573, 42.6949154942, 45.3711596574,
49.0308994631, 51.7466285605, 55.4583417674,
58.2832773380, 62.0948254963}

```

IRC - SP direction goes to gMin at 17.1276

```
SPweg = Join[Reverse[NT20DhalbIRCsp1], NT20DhalbIRCsp1vor]
```



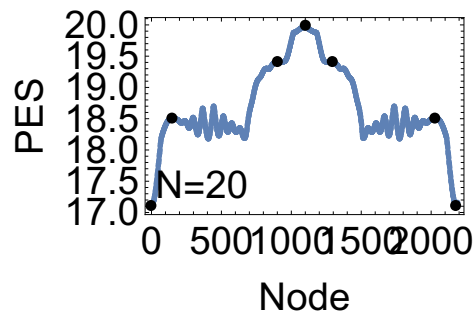
END point IRC

```

-0.73436092137125930 × 1.7331509332248058 × 5.1973393420202125 ×
7.7573920257457045 × 11.337072048185952 × 13.942298586645373 ×
17.565119291293570 × 20.186698414353401 × 23.826099990339461 ×
26.452426746871637 × 30.096241017744635 × 32.722567774276847
36.361969350262839 × 38.983548473322756 × 42.606369177970855 × 45.211595716430374 ×
48.791275738870532 × 51.351328422596104 × 54.815516831391456 × 57.283028685987546

```

node 146 energy = 18.5099 SP  
 node 900 energy = 19.4144 Min  
 node1091 energy = 19.9595 SP1 detHess - 2.517



start lower iMin

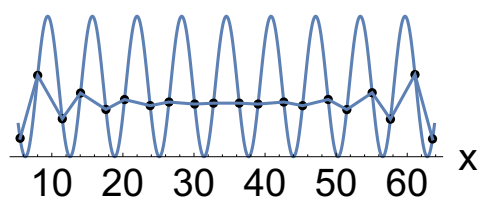
0.7395666461 × 4.5510355883 × 7.3754937710  
 11.0876454131 × 13.8040308017 × 17.4654410780  
 20.1442224172 × 23.7851259952 × 26.4508274959  
 30.0847722637 × 32.7472900747 × 36.3812851458  
 39.0471032955 × 42.6882063830 × 45.3673464836  
 49.0292870658 × 51.7466850358 × 55.4600725696  
 58.2874837432 × 62.1008137401 □

End is gMin ok but over a high summit ?

node 2178 energy 17.1242558

node2178 = {5.5402003373, 8.0126867224, 11.4726102930,  
 14.0441498572, 17.6113767148, 20.2333436238,  
 23.8378827324, 26.4802459601, 30.0977835161,  
 32.7470631366, 36.3677897398, 39.0169418008,  
 42.6343648730, 45.2762781059, 48.8802540178,  
 51.5011889053, 55.0665677550, 57.6358381964,  
 61.0904233873, 63.5594550682}

SetX = node2178



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

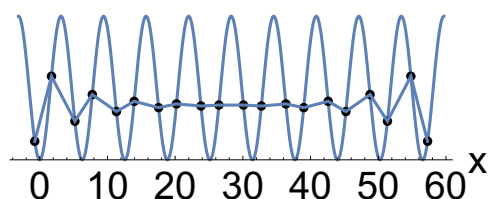
```
N = 20 a0 HALF minimum
```

```
ENERGY 17.12419893208451
```

```
SetX = {-0.73530148208424, 1.7354803959014, 5.1927324506611, 7.763148118761885,
  11.329441306608594, 13.95095242473732, 17.55517575532024,
  20.197359604363957, 23.81478347754269, 26.464001019105908,
  30.084666654324916, 32.7338841367429, 36.35130797203429,
  38.993491741050924, 42.5977150510515, 45.219226143493415,
  48.78551934599666, 51.3559351672787, 54.813187271401254, 57.28396915490723}
```

```
Eigenvalues
```

```
{4.21549, 4.14157, 4.02013, 3.85388, 3.64648, 3.40229,
  3.12636, 2.82654, 2.53449, 2.30966, 2.0535, 1.71852, 1.40229,
  1.1185, 0.868649, 0.65577, 0.483351, 0.354846, 0.27405, 0.2432}
```



```
SP event by node70 ?
```

```
node693 energy = 19.4144 detHessian - 5.83
```

```
node693 = {0.6679144413, 4.4306103267, 7.2327438348,
  10.8480359714, 13.4741921569, 16.8885131908,
  19.3780188728, 22.3717311228, 24.9939819749,
  27.4779184262, 30.6767089894, 33.2017896645,
  36.7038324797, 39.3669642473, 43.0253897700,
  45.8664013182, 49.6587321425, 52.8808621247,
  56.6052543688, 60.3862030230}
```

```
Setxx = node693
```

```
Out[ ] = {0.66975, 4.43213, 7.23353, 10.8485, 13.4743, 16.8884,
  19.3777, 22.3709, 24.9934, 27.4771, 30.6762, 33.2012, 36.7032,
  39.3661, 43.0243, 45.8645, 49.6566, 52.8767, 56.6027, 60.3826}
```

```
Eigenvalues
```

```
Out[ ] = {4.22133, 4.15061, 4.03927, 3.88723, 3.70254, 3.51399, 3.26751,
  3.07183, 2.78063, 2.33961, 1.56356, 1.31265, 1.01844, 0.751581,
  0.583746, 0.387385, 0.269028, -0.230254, 0.212885, -0.0109923}
```

```
is SP index 2
```



```

node70 energy = 18.508762 detHess - 1199.62
node70 = {-0.6894884143, 1.7721991344, 5.2136736018,
7.7781821116, 11.3398192128, 13.9601257660,
17.5648014217, 20.2101088630, 23.8333964539,
26.4933013382, 30.1311878681, 32.8097106507,
36.4726076364, 39.1941900027, 42.9129071179,
45.7547167522, 49.5762691783, 52.7618913743,
56.5488588227, 60.3360173292}
Setxx = node70

SetX = {-0.7348049408221831, 1.7363452707831115, 5.1938235237862305,
7.764970208731917, 11.33215799167777, 13.955457322206389,
17.56229283553398, 20.20905533837042, 23.83357757977387,
26.494765695658028, 30.134240006577834, 32.81521626631089,
36.48152128497891, 39.20955766691434, 42.93577350990813, 45.79630110117102,
49.627399210943445, 52.862840395299735, 56.61604510294878, 60.43657618161917}

ENERGY 18.50996631625231

```

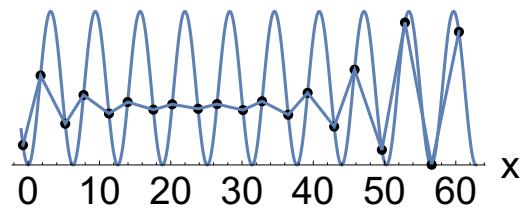
### Eigenvalues

```

{4.216997577874491, 4.146780906219639, 4.0307906721047395, 3.8734936945702496,
3.6832335733147676, 3.4706416585705004, 3.234224942582423,
2.9537056025795114, 2.619476164316755, 2.2884088087033216,
1.895215099801781, 1.516887816284847, 1.1979145796855248, 0.926298360368798,
0.6983838057357432, 0.5122051431337931, 0.36835013530771343,
0.27304592061054, 0.23789133544776098, -0.2058115207205251}

```

SP1 ENERGY 18.509966316252317`



SP20Da0HALF

### Search mirror SP

Umkehr = -SetX

SPmirror = Reverse[Umkehr] + 20. \* Pi

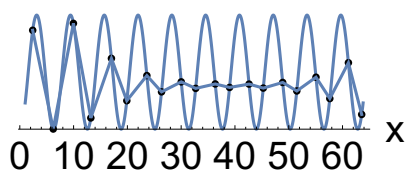
```

{0.734805, -1.73635, -5.19382, -7.76497, -11.3322, -13.9555,
-17.5623, -20.2091, -23.8336, -26.4948, -30.1342, -32.8152, -36.4815,
-39.2096, -42.9358, -45.7963, -49.6274, -52.8628, -56.616, -60.4366}

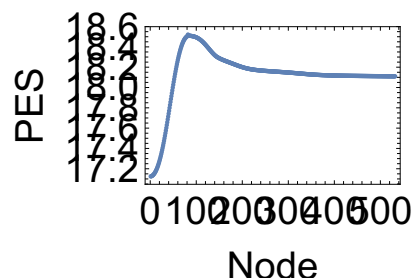
{2.39528, 6.21581, 9.96901, 13.2045, 17.0356, 19.8961,
23.6223, 26.3503, 30.0166, 32.6976, 36.3371, 38.9983, 42.6228,
45.2696, 48.8764, 51.4997, 55.0669, 57.638, 61.0955, 63.5667}

```

SetX = SPmirror



SPweg = Join[Reverse[NT20DhalbIRCsp], NT20DhalbIRCsp2]



End Point of IRC

```
IRC691 = {-0.713966369636, 1.77037284082180, 5.2412157506871564,
  7.83637840115320, 11.446988145995759, 14.137002201184435,
  17.8505520883442, 20.694899113732149, 24.530671358755605,
  27.7648021923466, 31.517329038607418, 35.331024842458326,
  38.4762859563196, 42.289814708475539, 45.138168629634563, 48.8768110138164,
  51.653218295024288, 55.396933691664948, 58.2400151730050, 62.0695151850634}
```

Setxx =

IRC691

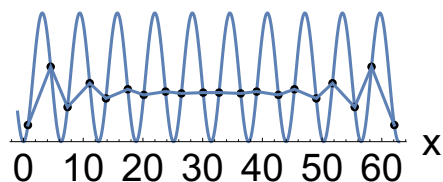
ENERGY 17.12419893208379

```
SetX = {0.73530136070908, 4.5477047700919, 7.373638054865044,
  11.086407545721519, 13.803299589691134, 17.46497371343183,
  20.143935755654205, 23.784937345310944, 26.45069886723791,
  30.08466660813462, 32.74718634366922, 36.38115402038136, 39.04691549429292,
  42.68791699023727, 45.366879058907465, 49.02855334709441,
  51.745445353072654, 55.45821489780775, 58.284148106598764, 62.09655151738705}
```

Eigenvalues

```
{4.21549, 4.14157, 4.02013, 3.85388, 3.64648, 3.40229,
  3.12636, 2.82654, 2.53449, 2.30966, 2.0535, 1.71852, 1.40229,
  1.1185, 0.868649, 0.65577, 0.483351, 0.354846, 0.27405, 0.2432}
```

SD goes to intMinimum but same ENERGY as gMin



iMinHalf

```

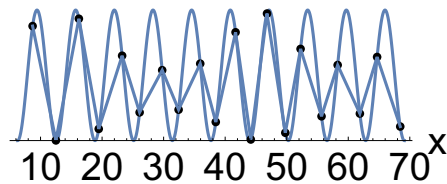
SP by node79 energy = 19.5247 detHess - 36.249
node79 = {2.3420755525, 6.1973462866, 9.9668833764,
13.2204797820, 17.0825287166, 19.9637692278,
23.7425739641, 26.5376478230, 30.3189935063,
33.2105271848, 37.0771210372, 40.3610606075,
44.1064634559, 47.9757138050, 51.0924811891,
54.9451511406, 57.7983563532, 61.6004479443,
64.4595820173, 68.3170958665}

```

```

Min energy = 19.4146 detHess 13.3788
node542 = {8.7098705270, 12.4982697764, 16.2282409571,
19.4568474169, 23.2567717784, 26.0996029301,
29.7663662115, 32.4323072165, 35.9483011257,
38.4724790569, 41.6907362241, 44.1628469869,
46.7970514399, 49.7714117204, 52.2531154034,
55.6569238428, 58.2776866254, 61.8878909929,
64.6874880318, 68.4469803960}
SetX = node542

```



```

-----
test iMin by node 345 : no grad min on NT
node345 = {-0.6094299415, 2.6418837354, 6.3724179774,
10.1920688421, 13.3174991124, 17.125473775,
19.9451225534, 23.6540444644, 26.3672013957,
30.0243726182, 32.6975611443, 36.3292504751,
38.9810433029, 42.5914042175, 45.2178315164,
48.7886147759, 51.3635435526, 54.8290018485,
57.3046422194, 60.4670334654 }
N = 20 HALF minimum
Setxx = node345

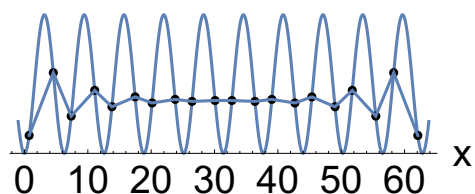
ENERGY 17.124198932083736

SetX = {0.735301497797181, 4.5477049368812335, 7.373638173265087,
11.086407677110838, 13.80329969764284, 17.46497383723436,
20.143935806450813, 23.784937377509117, 26.450698914615007,
30.084666679689153, 32.747186392106705, 36.38115415718085,
39.046915694286746, 42.68791726534505, 45.3668792345615, 49.02855337415303,
51.74544539468503, 55.45821489853078, 58.28414813491463, 62.09655157399869}

```

## Eigenvalues

```
{4.21549, 4.14157, 4.02013, 3.85388, 3.64648, 3.40229,
 3.12636, 2.82654, 2.53449, 2.30966, 2.0535, 1.71852, 1.40229,
 1.1185, 0.868649, 0.65577, 0.483351, 0.354846, 0.27405, 0.2432}
```



```
globSP node200 energy = 19.5238 detHess 3.23
```

```
? BBP point crossed ?
```

```
node199 = {0.7746991481, 4.6157929379, 7.4615483649,
11.2312847183, 14.0286720030, 17.8201784658,
20.7547045803, 24.6338506255, 28.0345365320,
31.6727124276, 35.5648356881, 38.6114861857,
42.4489673225, 45.2869323166, 49.0890776979,
51.9669793351, 55.8345148962, 59.0419218612,
62.8463315569, 66.6514887255}
```

```
next grad Min node283
```

```
next flat iMIN node345 energy = 19.268 detHess 17.049
```

```
node346 = { 0.9111399471, 4.8262866805, 7.7498384055,
11.6619435357, 14.7811393818, 18.7067817016,
22.4771315819, 25.7934601500, 29.7125289024,
32.6426675941, 36.5100929839, 39.4442314627,
43.3633081169, 46.6993847326, 50.4506231106,
54.3846000893, 57.4932759125, 61.4060649895,
64.3383940141, 68.2566256145}
```

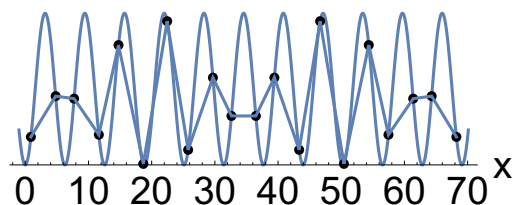
```
Setxx = node346
```

```
ENERGY 19.26838320922749
```

```
SetX = {0.8881371477214336, 4.805627699584506, 7.727461832729592,
11.641303006475152, 14.756482730083782, 18.685938270506526,
22.452505210833746, 25.77390883629086, 29.69344402889791,
32.624461528708835, 36.490576850266564, 39.42159435007747,
43.34112954268451, 46.66253316814157, 50.42910010846885, 54.35855564889159,
57.47373537250026, 61.38757654624583, 64.30941067939094, 68.226901231254}
```

## Eigenvalues

```
{4.22542925752079, 4.157755589884258, 4.037186673666635, 3.8740714494592012,
 3.6918262489333635, 3.5057083587792697, 3.2030417914641554,
 2.8944153432259245, 2.860394642863999, 2.194706209639527, 1.6745585774463088,
 1.6572923198643417, 1.1574117846335743, 0.8260925898372142,
 0.7097763074440566, 0.5312353525032218, 0.36086069183846536,
 0.3084390818654068, 0.04683871274552498, 0.01760839349850407}
```



ENERGY iMinOBEN 19.2684

```
### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

N = 20 Half search SP2 -> is index 4

```
SetX = {2.1604920338265355`*^-13, 3.141592653590432, 6.28318530718001,
 9.424777960770012, 12.566370614359379, 15.707963267948955,
 18.849555921538542, 21.991148575127912, 25.132741228717922,
 28.27433388230751, 31.415926535897725, 34.55751918948774,
 37.69911184307774, 40.84070449666795, 43.98229715025753, 47.12388980384754,
 50.2654824574369, 53.407075111026494, 56.54866776461607, 59.69026041820543}
```

Eigenvalues

```
{4.214071596084984, 4.148961141749635, 4.043421274379061, 3.9021130325903073,
 3.7320508075688776, 3.5433619184268172, 3.3507144388859746,
 3.175570504584947, 3.047801015178786, 2.4142135623730967, 0.9521989848212162,
 0.8244294954150564, 0.6492855611140262, 0.45663808157318453,
 -0.414213562373096, 0.26794919243112547, -0.214071596084979,
 -0.148961141749631, 0.09788696740969449, -0.043421274379059405}
```

SP\_4 at > 19.9, SP1 or so at 19.425

' maximum' at energy 19.9591982 SP3 detHess - 2.5172

```
node1091 = {3.5081108918, 6.2892793701, 9.0765418737,
 12.2050446805, 14.9800326267, 18.4203467481,
 21.4445090316, 24.9884907266, 28.3887216650,
 31.6748141100, 35.2169119107, 38.1463727180,
 41.5083309934, 44.2511654325, 47.2596404211,
 50.1327813490, 52.8736102943, 56.1229590087,
 58.9593413410, 62.4632778994}
```

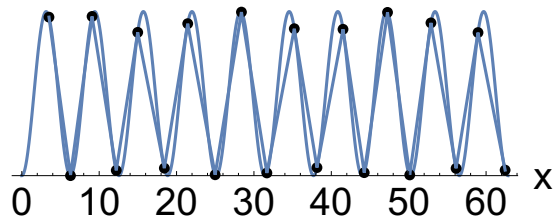
Setxx = node1091

```
SetX = {3.51149332083176, 6.2915631548873, 9.080010738646383,
 12.20643592894659, 14.980648014437968, 18.419726729624724,
 21.442089907162607, 24.98633757352911, 28.384704027884542,
 31.672924280478643, 35.21532258117273, 38.14634081117319, 41.50982774086336,
 44.25301614229993, 47.263628855027875, 50.13495685355449,
 52.876129558610955, 56.12365120806944, 58.95883699218557, 62.46195243599526}
```

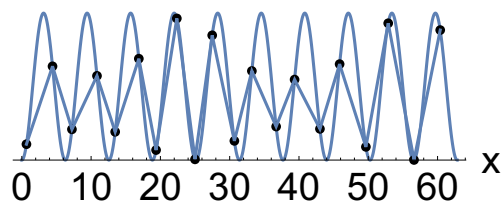
ENERGY SP3 19.959509261652

## Eigenvalues

```
{4.2176572497037705, 4.151386373809494, 4.0437469750461545,
 3.8997232888051423, 3.724805998946204, 3.530614788057072, 3.351623531892123,
 3.138649427614431, 3.0016902319915784, 2.39274905430518, 1.0895841101733375,
 0.9556789033266453, 0.7516121429408633, 0.5519431904876515,
 0.3614921580783297, -0.3558577886260972, 0.185736070122625,
 -0.137855576982941, 0.08043348952279583, -0.073835215427283}
```



sp3Half



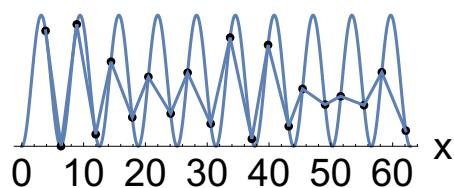
sp2at19p4145Half

```
SetX = {3.846738829954888, 6.340186331324868, 8.890603994690538,
 11.9501519125562, 14.431746333569683, 17.870265099652332,
 20.478681732251342, 24.085397682775287, 26.826015241371262,
 30.559141779493128, 33.705947584687436, 37.21878660102551,
 39.84731783189444, 43.17935862851082, 45.42872533952752, 49.06686170888567,
 51.59715139816022, 55.36022265054302, 58.249183866112276, 62.12632523893835}
```

## Eigenvalues

```
{4.23442, 4.16804, 4.03749, 3.8897, 3.69906, 3.50806, 3.25241,
 3.02341, 2.75156, 2.33254, 1.63597, 1.51696, 1.06685, 0.871483,
 0.635988, 0.46133, 0.322992, 0.254392, -0.224499, 0.101981}
```

ENERGY SP1 19.0379362957418



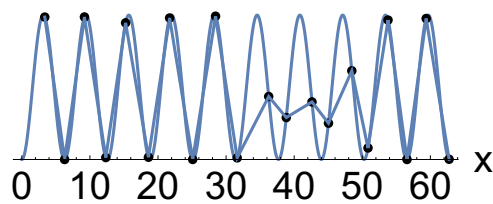
sp1at19p0379Half

SetX = {3.3758566867655535, 6.28532215612921, 9.196924472816304,  
 12.334413802792353, 15.242020765260705, 18.59889275910887,  
 21.70771830183588, 25.096194543558845, 28.448132235237782,  
 31.627145208501133, 36.256107400472, 38.8374635962721, 42.615353555885285,  
 45.03303940859354, 48.46348466080578, 50.838908529976095,  
 53.77891568663996, 56.56541167925724, 59.38172521845931, 62.74798836573337}

#### Eigenvalues

{4.29321, 4.15835, 4.07976, 3.90363, 3.76246, 3.52997, 3.37091,  
 3.12324, 2.79335, 2.41724, 1.74123, 1.05305, 0.875519, 0.623073,  
 0.466179, -0.390158, 0.324667, 0.148184, -0.103161, -0.068195}

SP  $2 \times 1/2$  ENERGY 20.27952565357851`



sp2andhalfat20p2795Half

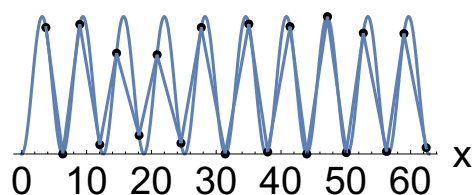
SP index  $2 \times 1/2$

SetX = {3.7150441615438297, 6.314102158547105, 8.944072081832475,  
 12.03644717659625, 14.623354990076256, 18.094383250114447,  
 20.879997100027243, 24.56182105837088, 27.70323850423388,  
 31.38520987477575, 35.02846657015974, 37.94235403484027, 41.38906613044271,  
 43.971819177055224, 47.16956214254261, 50.06612312361583,  
 52.69860115311202, 56.27341096747304, 58.97232943354094, 62.399330895202354}  
 {3.71504, 6.3141, 8.94407, 12.0364, 14.6234, 18.0944,  
 20.88, 24.5618, 27.7032, 31.3852, 35.0285, 37.9424, 41.3891,  
 43.9718, 47.1696, 50.0661, 52.6986, 56.2734, 58.9723, 62.3993}

#### Eigenvalues

{4.22986, 4.16119, 4.05938, 3.91149, 3.73749, 3.53116, 3.35415,  
 3.14463, 2.93269, 2.38572, 1.28191, 0.989766, 0.802133, 0.629079,  
 0.399066, -0.281957, 0.238066, 0.138776, -0.124645, -0.00243976}

SP  $2 \times 1/2$  ENERGY 20.07333403322829

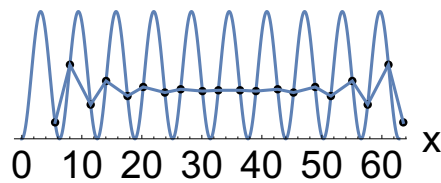


sp2andhalfat20p0733Half

```
SetX = {5.5478837071149725, 8.018665510691724, 11.475917689998447,
  14.046333621172666, 17.612626870168004, 20.23413796875697,
  23.838361342589042, 26.480545048736513, 30.097968754098694,
  32.7471862733139, 36.36785186980562, 39.017069349504204, 42.63449312478238,
  45.27667689033857, 48.88090016935289, 51.50241135411182, 55.0687046540876,
  57.63912053070794, 61.096372561630496, 63.56715448299631}
```

#### Eigenvalues

```
{4.21549, 4.14157, 4.02013, 3.85388, 3.64648, 3.40229,
  3.12636, 2.82654, 2.53449, 2.30966, 2.0535, 1.71852, 1.40229,
  1.1185, 0.868649, 0.65577, 0.483351, 0.354846, 0.27405, 0.2432}
```

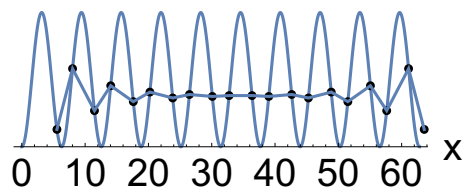


ENERGY 17.1241989320844

```
SetX = {5.547883809351418, 8.01866567741648, 11.47591774824249,
  14.046333551580352, 17.61262683824212, 20.234138005836744,
  23.838361343807147, 26.480545079935457, 30.097968850018024,
  32.74718639213653, 36.367851986918865, 39.01706952905577, 42.63449329918359,
  45.27667703538236, 48.880900373497575, 51.502411541255, 55.06870482834865,
  57.639120631841315, 61.096372703734296, 63.567154570700936}
```

#### Eigenvalues

```
{4.21549, 4.14157, 4.02013, 3.85388, 3.64648, 3.40229,
  3.12636, 2.82654, 2.53449, 2.30966, 2.0535, 1.71852, 1.40229,
  1.1185, 0.868649, 0.65577, 0.483351, 0.354846, 0.27405, 0.2432}
```





```

stat point energy = 19.41436 detHess 12.4646
is 'flat SP_2 NT is 'misleading' for MEP
node381 = {-0.6697271388, 1.8510934931, 5.3328873586,
8.0010923847, 11.6584960064, 14.5277019071,
18.3216129243, 21.6117656688, 25.2722641832,
29.0718304560, 32.1557812652, 35.9139017332,
38.6948993596, 42.3150442583, 44.9397563549,
48.3820565664, 50.8725211264, 53.9329626790,
56.4903446334, 58.9884405957}

```

```

stat energy = 19.9593276 detHess - 2.28549
is 'flat' SP_3
node616 = {-0.3698719336, 2.4102247687, 5.8582097761,
8.8938962659, 12.4358765759, 15.8477327870,
19.1202739105, 22.6602379974, 25.5799293401,
28.9320511255, 31.6728582507, 34.6677743104,
37.5526481762, 40.2915621926, 43.552393190,
46.3963719170, 49.9052213550, 53.0613316010,
56.5558215794, 60.0569884265}

```

```

stat energy = 19.999566 detHess 0.99 is SP_4
node713 = {0.0001871894, 3.1419671365, 6.2833726336,
9.4249655074, 12.5663709356, 15.7077768670,
18.8493695593, 21.9907765666, 25.1325569060,
28.2741554423, 31.4159373291, 34.5577393388,
37.6993395281, 40.8412016309, 43.9826356123,
47.1245302186, 50.2660460182, 53.4085172747,
56.5504639964, 59.6950541135}

```

```

nodes 805, 1037 go further on axis ok
node805 = {0.3698776995, 3.8729718532, 6.7081692770,
9.9556729007, 12.6968712706, 15.5682002799,
18.5788378682, 21.3220523529, 24.6855447634,
27.6165989090, 31.1589811812, 34.4472402536,
37.8455630819, 41.3898295271, 44.4121857863,
47.8513663346, 50.6256769648, 53.7526193857,
56.5412639701, 59.3228842619}

```

```

node1037 = {0.6697612228, 4.4321527629, 7.2335541488,
10.8485854986, 13.4744001945, 16.8885076362,
19.3778015911, 22.3711139947, 24.9935371309,
27.4772035758, 30.6762204429, 33.2011600412,
36.7031833282, 39.3659188507, 43.0240013426,
45.8637866826, 49.6555136669, 52.8741287851,
56.6001849802, 60.3771519727}

```

```
Setxx = node381
```

Eigenvalues

```

Out[*]= {4.22133, 4.15061, 4.03927, 3.88723, 3.70254, 3.51399, 3.26751,
3.07183, 2.78063, 2.33961, 1.56356, 1.31265, 1.01844, 0.751581,
0.583746, 0.387385, 0.269028, -0.230254, 0.212885, -0.0109923}

```

**Setxx = node616**

Out[\*]= {-0.369901, 2.41017, 5.85817, 8.89383, 12.4358, 15.8477,  
19.1203, 22.6603, 25.58, 28.9321, 31.6729, 34.6679, 37.5527,  
40.2916, 43.5525, 46.3966, 49.9055, 53.0623, 56.557, 60.0602}

**Eigenvalues**

Out[\*]= {4.21766, 4.15139, 4.04375, 3.89972, 3.72481, 3.53061, 3.35162,  
3.13865, 3.00169, 2.39275, 1.08958, 0.955679, 0.751612, 0.551943,  
0.361492, -0.355858, 0.185736, -0.137856, 0.0804335, -0.0738352}

**Setxx = node713**

Out[\*]= { $1.9962 \times 10^{-13}$ , 3.14159, 6.28319, 9.42478, 12.5664, 15.708,  
18.8496, 21.9911, 25.1327, 28.2743, 31.4159, 34.5575, 37.6991,  
40.8407, 43.9823, 47.1239, 50.2655, 53.4071, 56.5487, 59.6903}

**Eigenvalues**

Out[\*]= {4.21407, 4.14896, 4.04342, 3.90211, 3.73205, 3.54336, 3.35071,  
3.17557, 3.0478, 2.41421, 0.952199, 0.824429, 0.649286, 0.456638,  
-0.414214, 0.267949, -0.214072, -0.148961, 0.097887, -0.0434213}

**stat energy = 19.89727 detHess 230.04 SP2**

node381 = {2.3964759484, 6.2178265330, 9.9738648663,  
13.2079946239, 17.0406216460, 19.9014697629,  
23.6306917883, 26.3622759504, 30.0361932988,  
32.7283077410, 36.3872183887, 39.0794575899,  
42.7536158304, 45.4857268411, 49.2155695779,  
52.0780324410, 55.9114149368, 59.1498077371,  
62.9027247449, 66.7264541117}

**stat energy = 19.526226 detHess - 38.895 SP1**

node600 = {2.3552259501, 6.2064663803, 9.9810631201,  
13.2276247377, 17.0882934725, 19.9670461102,  
23.7448028755, 26.5392316272, 30.3201924995,  
33.2118891396, 37.0783427763, 40.3631354972,  
44.1075497471, 47.9768893523, 51.0929722836,  
54.9452902075, 57.7981388527, 61.5998052068,  
64.4583002620, 68.3152472076}

**Setxx = node381**

Out[\*]= {2.39253, 6.21508, 9.96956, 13.2058, 17.0388, 19.9005,  
23.63, 26.3619, 30.0359, 32.7281, 36.387, 39.0792, 42.7532,  
45.485, 49.2146, 52.0762, 55.9092, 59.1455, 62.9, 66.7225}

**Eigenvalues**

{4.218404641576897, 4.151668878828522, 4.040715931876176, 3.8911257984732894,  
3.7139264663201224, 3.5229661420279266, 3.3192920864636424,  
3.07629687729177, 2.749161909514733, 2.2206738673901385, 1.6717369709905103,  
1.2942902963638203, 0.9923987509443677, 0.7464126780176241,  
0.5461705190844368, 0.38656699571521136, 0.2728856337863683,  
0.23471723712651027, -0.20457369487140578, -0.20454783419384}

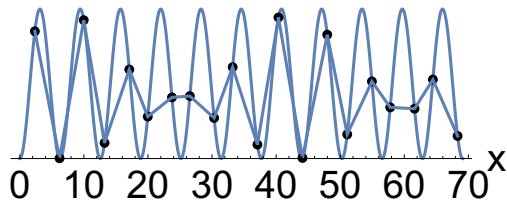
Setxx = node600

SetX = {2.350500052885901, 6.203213941122733, 9.976041473358658,  
13.225104953409064, 17.08628501215862, 19.96593139243741,  
23.744093390144794, 26.5387988869504, 30.319965965837643, 33.21176562126712,  
37.07835046012286, 40.363281318958904, 44.10770546055951,  
47.97721019716573, 51.093248193693974, 54.945708372390804,  
57.798686123445314, 61.60065453426473, 64.45973439699391, 68.31718549530314}

Eigenvalues

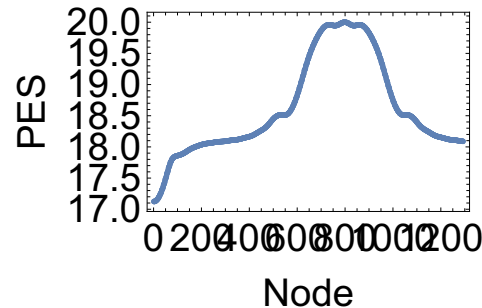
Out[ ] = {4.22286, 4.15234, 4.03739, 3.88836, 3.70291, 3.48875, 3.31249,  
3.01457, 2.72478, 2.20293, 1.83961, 1.34283, 1.03392, 0.848208,  
0.589728, 0.447008, 0.310722, 0.259604, -0.185438, 0.0197937}

SP1 ENERGY 19.52473724672591



SP1at19p5247

NT start iMin with (1, 1, ..., 1, 1)



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

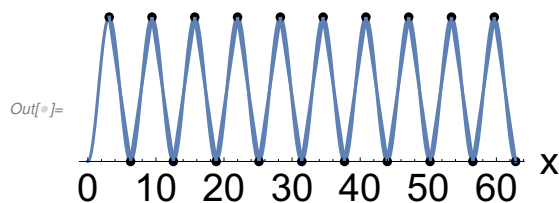
N = 20 a0 HALF global SP a0 + Pi

Setxx = Table[a0 \* (i - 1) + Pi, {i, 20}]

SetX = {3.141592653590426, 6.283185307179793, 9.424777960769367,  
12.566370614358954, 15.707963267948319, 18.849555921538332,  
21.991148575127916, 25.13274122871814, 28.274333882308152,  
31.415926535898155, 34.55751918948838, 37.69911184307796,  
40.84070449666796, 43.98229715025732, 47.12388980384689, 50.26548245743648,  
53.40707511102584, 56.54866776461585, 59.69026041820543, 62.83185307179565}

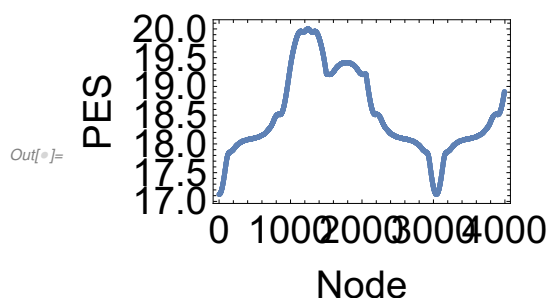
## Eigenvalues

Out[ ]= {4.21407, 4.14896, 4.04342, 3.90211, 3.73205, 3.54336, 3.35071,  
3.17557, 3.0478, 2.41421, 0.952199, 0.824429, 0.649286, 0.456638,  
-0.414214, 0.267949, -0.214072, -0.148961, 0.097887, -0.0434213}



ENERGY 20.0

path direction 1, 1, ..., 1, 1



## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##

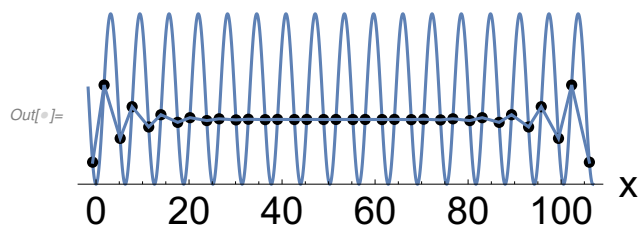
HALF N = 35 global minimum

ENERGY 30.28639064150825

{-0.73522, 1.73562, 5.19291, 7.76345, 11.3299, 13.9517, 17.5563, 20.1993, 23.8179,  
26.469, 30.0928, 32.7472, 36.3729, 39.0284, 42.6549, 45.3109, 48.9377, 51.5939,  
55.2209, 57.8773, 61.5045, 64.1612, 67.7888, 70.4463, 74.0751, 76.7345,  
80.3665, 83.0311, 86.6714, 89.3499, 93.0113, 95.728, 99.4407, 102.267, 106.079}

## Eigenvalues

Out[ ]= {4.23222, 4.20802, 4.16789, 4.11212, 4.04113, 3.95548, 3.85581, 3.74287, 3.6175,  
3.48063, 3.33326, 3.17646, 3.01152, 2.84034, 2.66711, 2.5021, 2.35618, 2.21254,  
2.04385, 1.85875, 1.67499, 1.4983, 1.33002, 1.17086, 1.02157, 0.882969, 0.755897,  
0.641171, 0.53956, 0.451781, 0.378505, 0.320382, 0.278066, 0.252106, 0.241785}



## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##

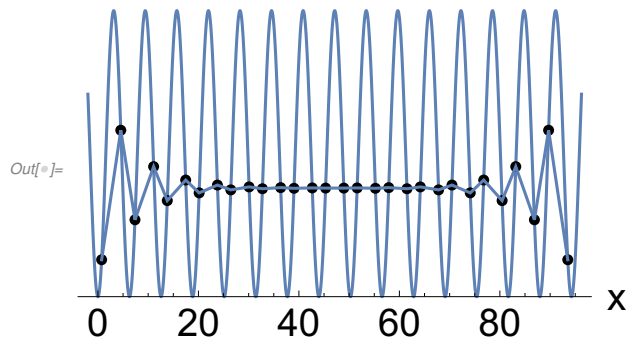
rs = 11 111 HALF N = 30 global Min a0

ENERGY 25.898979946339

Out[*n*]= {0.735221, 4.54756, 7.37346, 11.0861, 13.8029, 17.4642, 20.1428,  
23.783, 26.4476, 30.0797, 32.7391, 36.368, 39.0255, 42.6533, 45.3101,  
48.9376, 51.5945, 55.2223, 57.8798, 61.5087, 64.1681, 67.8001,  
70.4647, 74.105, 76.7835, 80.4449, 83.1617, 86.8743, 89.7002, 93.5126}

Eigenvalues

Out[*n*]= {4.22929, 4.19637, 4.14185, 4.0663, 3.97048, 3.85538, 3.72217, 3.57219,  
3.40689, 3.2279, 3.03708, 2.8373, 2.63584, 2.45164, 2.29217, 2.11455,  
1.90144, 1.68433, 1.47711, 1.28205, 1.10009, 0.932333, 0.780012,  
0.644378, 0.52662, 0.427846, 0.349108, 0.291471, 0.255965, 0.242083}

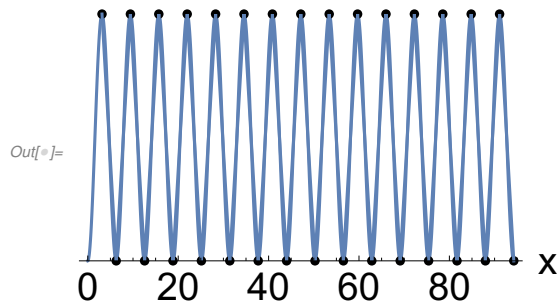


HALF N = 30 global SP a0 + Pi

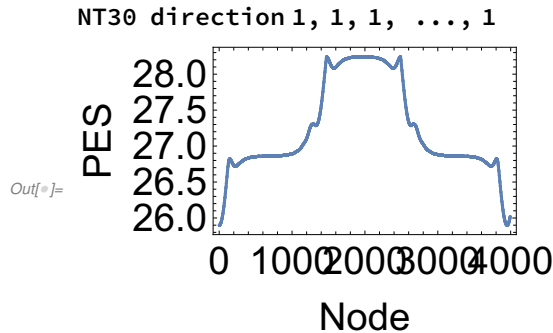
SetX = {3.14148760411095, 6.2831853071799, 9.42488301024938, 12.56647566383861,  
15.708173366906697, 18.84966097101785, 21.991253624607523,  
25.132741228718047, 28.2742288328282, 31.415821486418544, 34.55730909053,  
37.69900679359839, 40.840599447188225, 43.982297150257324,  
47.1239948533266, 50.265587506916034, 53.40728520998421, 56.54877281409545,  
59.6903654676853, 62.83185307179574, 65.97334067590604, 69.11493332949614,  
72.2564209336075, 75.39811863667582, 78.53971129026549, 81.68140899333467,  
84.82310669640393, 87.96469934999348, 91.10639705306174, 94.24788465717305}

Eigenvalues

Out[*n*]= {4.22627, 4.19706, 4.14896, 4.08285, 4., 3.90211, 3.79138, 3.67061, 3.54336,  
3.41421, 3.28908, 3.17557, 3.08301, 3.02162, 2.41421, 0.978381, 0.916991,  
0.82443, 0.710916, 0.585786, 0.456638, -0.414214, 0.329388, -0.226274,  
0.208616, -0.197064, -0.148961, 0.097887, -0.0828493,  $1.10354 \times 10^{-8}$ }



ENERGY 30.0



is the cape Start at

```

0.735221 × 4.547560 × 7.373460 × 11.086100
13.802900 × 17.464200 × 20.142800 × 23.78300
26.447600 × 30.079700 × 32.739100 × 36.36800
39.025500 × 42.653300 × 45.310100 × 48.93760
51.594500 × 55.222300 × 57.879800 × 61.50870
64.168100 × 67.800100 × 70.464700 × 74.10500
76.783500 × 80.444900 × 83.161700 × 86.87430
89.700200 × 93.512600
SP node468 to 482 energy26 .84863567 detHess - 6680.867
0.7372489306 × 4.5504937332 × 7.3762132498
11.0893542706 × 13.8062876894 × 17.4683764479
20.1477869600 × 23.7896792321 × 26.4567893642
30.0930095813 × 32.7591931813 × 36.3990016591
39.0746207605 × 42.7306300778 × 45.4365287067
49.1350396288 × 51.9283477903 × 55.7168188711
58.7655103466 × 62.6120704220 × 66.2400112683
69.6039305515 × 73.4368962389 × 76.3445531999
80.0628834086 × 82.7817507192 × 86.3913786208
89.0004077256 × 92.4691124546 × 94.9587429146
node541 - 475 ...
node625 ...
node1844 energy = 28.23424391 detHess - 1539.689
2.4015510163 × 6.2180020754 × 9.9698557113
13.2037644309 × 17.0333158167 × 19.8933772734
23.6183107610 × 26.3453720423 × 30.0095144737
32.6876772602 × 36.3219978036 × 38.9755558599
42.5866438263 × 45.2135698212 × 48.7839488884
51.3588488904 × 54.8224673650 × 57.2986764296
60.4570702536 × 62.9221622898 × 65.4779804968
68.5097793495 × 70.9731427519 × 74.3960559864
76.9768686600 × 80.5581901925 × 83.2385532322
86.9193627429 × 89.7356711788 × 93.5325300763
node1900 energy = 28.2415927 detHess 3051.012
2.4029554297 × 6.2184061759 × 9.9697001738
13.2032196872 × 17.0319814230 × 19.8916157608
23.6152723145 × 26.3409275245 × 30.0021340114
32.6762173848 × 36.3030570926 × 38.9457023875
42.5368287972 × 45.1363755697 × 48.6509217565

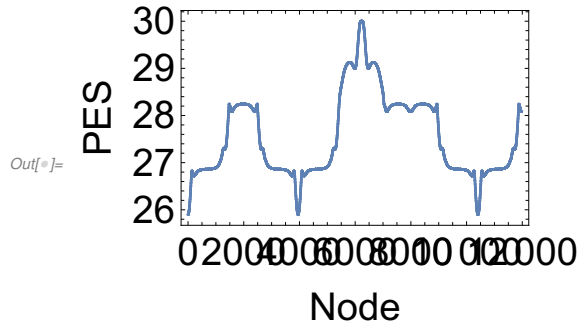
```

```

51.1670025373 × 54.4679313058 × 56.8966634288
59.6669869399 × 62.4611589151 × 64.8936454508
68.2085727262 × 70.7367474659 × 74.2642035175
76.8861165352 × 80.5051721140 × 83.2016387764
86.8974043102 × 89.7178990417 × 93.5223623775
node 3994 energy = 26.020784743 detHess 802 006.95
5.6928926200 × 8.2341869426 × 11.6603755171
14.2558304568 × 17.8005589278 × 20.4346694642
24.0249832994 × 26.6769034502 × 30.2847747224
32.9440487611 × 36.5587181868 × 39.2208955864
42.8381778981 × 45.5014200387 × 49.1196331926
51.7830915756 × 55.4014416408 × 58.0644701577
61.6822926778 × 64.3438367074 × 67.9599575578
70.6175565946 × 74.2291313751 × 76.8766158618
80.4761399101 × 83.0980343147 × 86.6643736791
89.2234016538 × 92.6904603499 × 95.1139156486

```

```
Join[NT30globSP111, NT30globSP111Teil2, NT30globSP111Teil3]
```



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

```
rs = 11111 HALF N = 40 global Min a0
```

```
ENERGY 34.67380171899
```

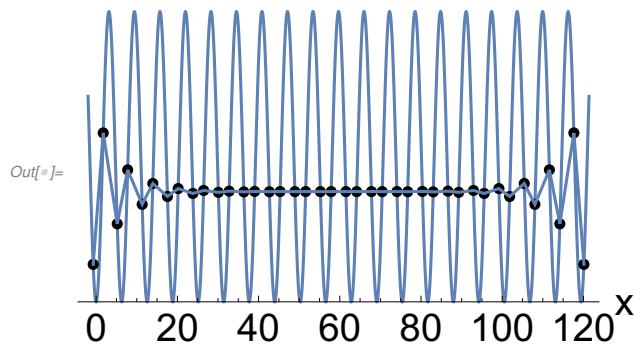
```

SetX = {-0.73522006140764, 1.7356221731799, 5.192911302134, 7.763446771251074,
11.32988685084115, 13.95169080975879, 17.556343400729226,
20.199275399488222, 23.817869186621, 26.469033063124183,
30.09282659880717, 32.7471405350399, 36.372891711404776,
39.02840265088169, 42.6548927352716, 45.31085675834642, 48.93762470253148,
51.59375734598939, 55.220625449280966, 57.87681363682262,
61.5037065337907, 64.15989494080111, 67.78676314257655, 70.44289583792768,
74.06966371865786, 76.72562760792495, 80.35211787585699, 83.00762884499441,
86.63337986217084, 89.2876937148695, 92.91148721816684, 95.56265120779307,
99.18124510527058, 101.82417729432109, 105.42882975383623, 108.05063388393,
111.61707402901273, 114.18760965381139, 117.64489870861, 120.1157409478489}

```

## Eigenvalues

```
Out[ ]= {4.23411, 4.21558, 4.18482, 4.14199, 4.08736, 4.02123, 3.944, 3.85612, 3.75811,
  3.65053, 3.534, 3.40916, 3.27674, 3.1375, 2.99235, 2.84262, 2.6909, 2.54306,
  2.40771, 2.28163, 2.14449, 1.98906, 1.82733, 1.66809, 1.51411, 1.36626,
  1.22507, 1.09109, 0.964882, 0.847045, 0.738158, 0.638776, 0.549428,
  0.470601, 0.402752, 0.346318, 0.301723, 0.269379, 0.249575, 0.241565}
```



```
### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

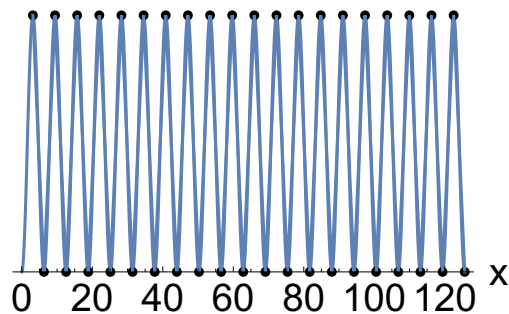
```
rs = 11 111 HALF N = 40 global SP a0 + Pi
```

```
Setxx = Table[a0 * (i - 1) + Pi, {i, 40}]
```

```
{3.14159, 6.28319, 9.42478, 12.5664, 15.708, 18.8496, 21.9911, 25.1327,
  28.2743, 31.4159, 34.5575, 37.6991, 40.8407, 43.9823, 47.1239, 50.2655,
  53.4071, 56.5487, 59.6903, 62.8319, 65.9734, 69.115, 72.2566, 75.3982,
  78.5398, 81.6814, 84.823, 87.9646, 91.1062, 94.2478, 97.3894, 100.531,
  103.673, 106.814, 109.956, 113.097, 116.239, 119.381, 122.522, 125.664}
```

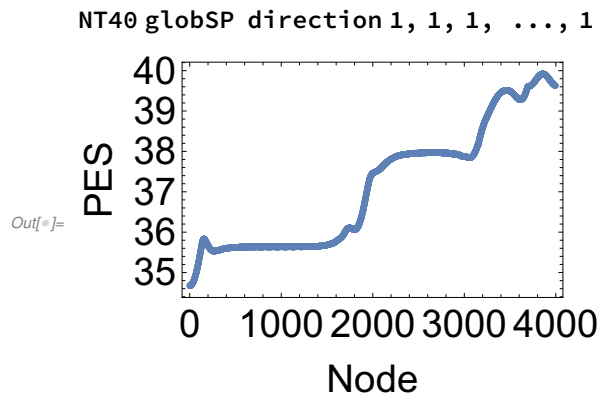
```
Eigenvalues
```

```
Out[ ]= {4.23056, 4.21407, 4.18678, 4.14896, 4.101, 4.04342, 3.97686, 3.90211, 3.82013,
  3.73205, 3.63925, 3.54336, 3.44638, 3.35071, 3.25928, 3.17557, 3.10362, 3.0478,
  3.01224, 2.41421, 0.987763, 0.952199, 0.896376, 0.824429, 0.74072, 0.649286,
  0.553619, 0.456638, -0.414214, 0.360753, 0.267949, -0.230555, -0.214072,
  -0.186781, 0.179871, -0.148961, -0.101003, 0.097887, -0.0434213, 0.0231386}
```



```
Energy 40.0
```





ok goes up to 40 in energy