

W.Quapp and J.M.Bofill

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

Supplementary Material 2

MF 2/3 N = 25, ... 35

```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
N = 25 a_o minimum

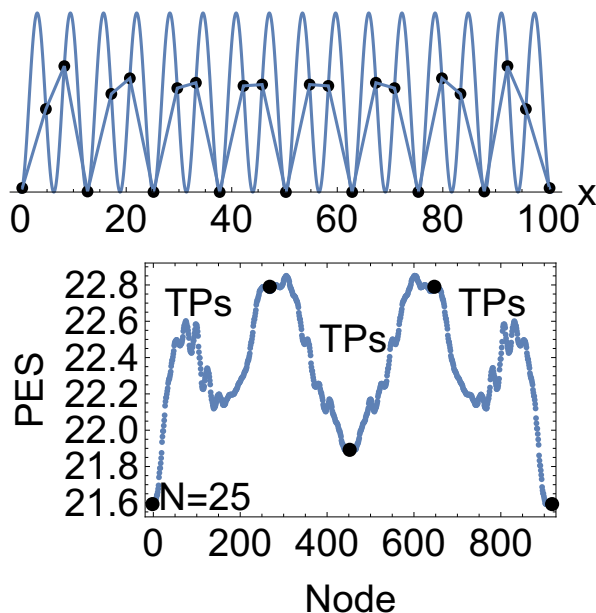
k = 1.0
as = 6.283185307180
a0 = 4.188790204787
Setxx = Table[a0 * (i - 1), {i, 25}]
SetAA = Table[A[i], {i, 25}]
SetXX = Setxx + SetAA
The formula for the FK model for N = 25
VVV = Sum[1 - Cos[SetXX[[i]]], {i, 25}] +
Sum[k/2. * (SetXX[[i + 1]] - SetXX[[i]] - a0)^2, {i, 24}]
GGG = Table[D[VVV, A[i]], {i, 25}]
Set00 = Table[-0.172, {i, 25}]
Set22 = Table[0.172, {i, 25}]
SetAA00 = Riffle[SetAA, Set00]
SetA0 = Partition[SetAA00, 2]
SetAA22 = Riffle[SetA0, Set22]
SetFl = Flatten[SetAA22]
SetFin = Partition[SetFl, 3]
G2G2G2 = Sum[GGG[[i]]^2, {i, 25}]
NMinimize[VVV, SetFin]
HHH = Table[D[GGG, A[j]], {j, 25}]

ENERGY 21.592494514373

SetXX = {0.30050064597104764, 4.785289305728147, 8.272734017600545,
12.673775687638496, 17.18201604856665, 20.694932417632025,
25.17038790324588, 29.68348117142048, 33.209611220122355,
37.711004323115674, 42.22428962582141, 45.75504782268725, 50.26548245743669,
54.77591709218613, 58.30667528905197, 62.819960591757706, 67.32135369475102,
70.8474837434529, 75.3605770116275, 79.83603249724136, 83.34894886630673,
87.85718922723488, 92.25823089727284, 95.74567560914524, 100.23046426890234}
```

Eigenvalues

```
{4.30363, 4.25848, 4.18659, 4.09019, 3.97395, 3.84778, 3.73694, 3.21888, 3.21565,
 2.71577, 2.53228, 2.31585, 2.08815, 1.86132, 1.64804, 1.45489, 1.42815,
 0.765863, 0.650425, 0.514666, 0.389611, 0.284872, 0.204366, 0.149853, 0.120649}
```



```
1. SP by node256 energy 22.78946 detHess - 1546.95
node256 = {0.8358265194, 5.7695859465, 10.2028372577,
13.9408246307, 18.6562241002, 23.1677026236,
26.7630115617, 31.3555004154, 35.8748500895,
39.4306919786, 43.9750406862, 48.4983564810,
52.0440274801, 56.5707143673, 61.1055346189,
64.6565618155, 69.1779926362, 73.7494563853,
77.3237562641, 81.8410002628, 86.5056014514,
90.1672405248, 94.6472121720, 99.5071463458,
103.4965359789}
```

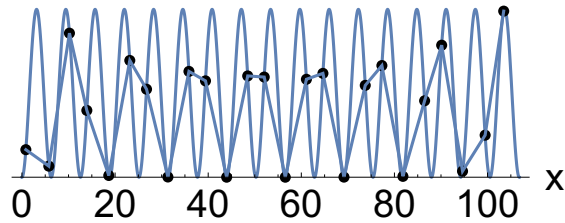
```
G2G2G2 = Sum[GGG[[i]]^2, {i, 25}]
NMinimize[G2G2G2, SetFin]
```

```
SetXX = {0.8340682428638276, 5.763529263087184, 10.196408666386363,
13.931983056197103, 18.646580981036294, 23.15959481876165,
26.752465370589388, 31.344139195641763, 35.864087322964735,
39.418741093548995, 43.962339674349714, 48.48598210406323,
52.03132428196297, 56.55770531245913, 61.0931237677716, 64.6426098581513,
69.16344332149002, 73.73266282711732, 77.30636913178236,
81.82371082314539, 86.48287456616016, 90.14600300625823,
94.62842849856322, 99.48237698415194, 103.4696057134984}
```

```
ENERGY 22.789510391639
```

Eigenvalues

```
{4.31007, 4.27239, 4.20696, 4.11869, 4.01321, 3.89731, 3.78025, 3.69118, 2.79363,
 2.68388, 2.50293, 2.29514, 2.07767, 1.86061, 1.65484, 1.50429, 1.21055,
 0.697748, 0.546996, 0.408854, -0.381208, 0.291612, 0.199433, 0.136983, 0.10018}
```



```
node434 iMin - double - min flat SP in between
energy = 21.891727 detHess 116.146
```

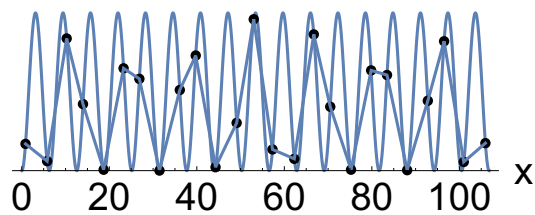
```
node434 = {0.8542237220, 5.7919829877, 10.2580558597,
13.9839891544, 18.6982136529, 23.2616729575,
26.8698761734, 31.4642769898, 36.1070094236,
39.7499688237, 44.2798951362, 49.1030460734,
53.0084236793, 57.3019771602, 62.2795871119,
66.7325793919, 70.4972784349, 75.2442533506,
79.8378655691, 83.4684432641, 88.0757324926,
92.7939312635, 96.5189606593, 101.0085843392,
105.9578743298}
```

```
ENERGY 21.89170076130546
```

```
SetXX = {0.8489928714599377, 5.788398412622624, 10.252959839421237,
13.980818120100434, 18.696478801735264, 23.259659496122307,
26.868181579288684, 31.46318042522583, 36.10541557668252,
39.7479129202978, 44.27832478521254, 49.10045958988925, 53.00379702974519,
57.299570026998445, 62.27764168207395, 66.72944044095387, 70.49522644728643,
75.24290163205804, 79.83587853238868, 83.46635807404937, 88.07399441701816,
92.79081278324848, 96.51410273497362, 101.0051089265717, 105.9526921737256`}
```

Eigenvalues

```
{4.32874, 4.27882, 4.21444, 4.12232, 4.00421, 3.91373, 3.73639, 3.7179, 2.91043,
 2.71972, 2.54416, 2.32896, 2.09216, 1.89598, 1.61525, 1.52432, 1.1891,
 1.17204, 0.519832, 0.453254, 0.29586, 0.212774, 0.132869, 0.112372, 0.0140472}
```

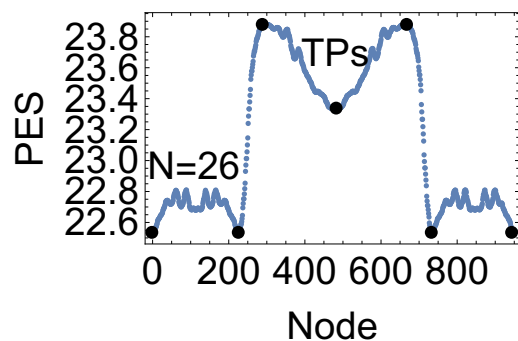
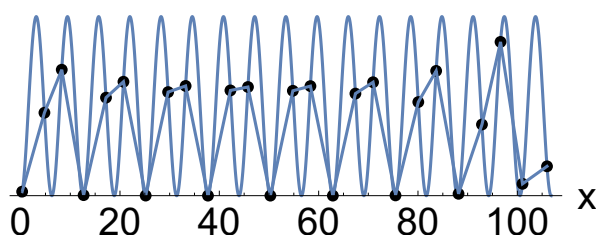


```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

```
N = 26 a_o minimum
```

```
ENERGY 22.535705537698018
```

```
SetXX = {0.3007336899189349, 4.78574494251626, 8.27344553741148,
12.67445354037529, 17.183334156239884, 20.69676432533082,
25.172235287474887, 29.687190042164563, 33.21459143916001,
37.71614293578557, 42.234724701796665, 45.768890719188356,
50.27986273076475, 54.80521452005278, 58.34543452421564, 62.86023166674755,
67.40340359529291, 70.95647687656337, 75.47314956835174, 80.06467805776244,
83.65726135582582, 88.16892497049642, 92.88350038461522,
96.61932477329583, 101.05131849195193, 105.9804991583565`}
```



```
next unsymm gMin by 227 energy = 22.53674
```

```
node227 = {0.8595869722 × 5.7870223119 × 10.2223278925 ×
13.9534383148 × 18.6640807718 × 23.1790604950 ×
26.7683622168 × 31.3570718767 × 35.8740721947 ×
39.4258933594 × 43.9683228059 × 48.4819566313 ×
52.0220898471 × 56.5485156346 × 61.0594395231 ×
64.5926567290 × 69.1115563765 × 73.6131010251 ×
77.1407288328 × 81.6552490019 × 86.1310646524 ×
89.6469860833 × 94.1566461555 × 98.5632278183 ×
102.0489838095 × 106.5370446175}
```

```
iMin by 472 energy = 23.3390 detHess 5.502286
```

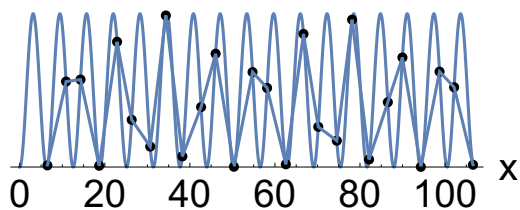
```
node472 = {6.4891078284, 10.8814720555, 14.2803388814,
18.6689741016, 22.8780073587, 26.3119498167,
30.6701965294, 34.3499349935, 38.2357700204,
42.6328718633, 46.0543763753, 50.3528476732,
54.7385730909, 58.1527939876, 62.5664594955,
66.7178359178, 70.1916889170, 74.5459160829,
78.1473418658, 82.1312435613, 86.5499618221,
89.9808488963, 94.3141492757, 98.7137706081,
102.1435946504, 106.5725438045}
```


ENERGY 23.33846009788914

```
SetXX = {6.487897681406666, 10.879973434509504, 14.278723528512094,
  18.667471208138167, 22.87513867272742, 26.309531105325064,
  30.66730197276256, 34.34444111647414, 38.23304961831374, 42.63058507348011,
  46.05202364476318, 50.351557180545456, 54.73705919290285, 58.15141662355354,
  62.565263615479594, 66.7156676983707, 70.19014467833033, 74.54426237378473,
  78.14449116607311, 82.12982826100186, 86.54870698135869, 89.97956012762181,
  94.31338112309626, 98.7127565907669, 102.14258260009858, 106.57157553347317`}
```

Eigenvalues

```
{4.27215, 4.22615, 4.17219, 4.07706, 3.96103, 3.83514, 3.67127, 3.56041, 3.13599,
  3.08874, 2.55497, 2.38179, 2.20841, 2.02651, 1.8275, 1.61012, 1.5602, 0.788536,
  0.633689, 0.575909, 0.41129, 0.285189, 0.221346, 0.167976, 0.0243102, 0.00492537}
```

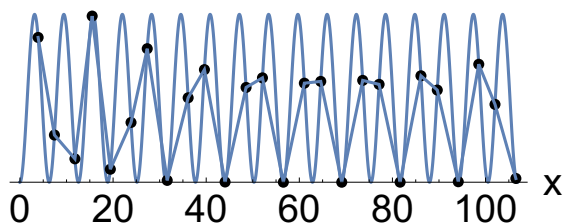


```
SP by node297 energy = 23.88109 detHess - 597.06
node297 = {3.9115732671, 7.4102826397, 11.8121619417,
  15.5293290908, 19.4241818906, 23.8625555590,
  27.3457733779, 31.6297497280, 36.1259236456,
  39.6221004234, 44.0568959385, 48.5662210709,
  52.0837864969, 56.5708779367, 61.0801777227,
  64.6057915661, 69.1108428979, 73.6116987609,
  77.1357339330, 81.6459044967, 86.1205780226,
  89.6323445084, 94.1394146474, 98.5383317891,
  102.0249104977, 106.5085376411}
```

```
SetXX = {3.900651494239602, 7.401202745120918, 11.80098890231161,
  15.50796275106159, 19.413606437190648, 23.853863774450527,
  27.33642770589061, 31.625313056356713, 36.122058265522, 39.61882305121696,
  44.05533208144665, 48.564811130895286, 52.0827120900751,
  56.57040172044066, 61.07982359561159, 64.60562329619212,
  69.11089441935444, 73.612021594756, 77.13625902521021, 81.64654457579186,
  86.12197277151184, 89.63411851473762, 94.14139461745876,
  98.54248628982359, 102.02954640804629, 106.51400016814281`}
```

Eigenvalues

```
{4.30074, 4.25367, 4.18531, 4.09795, 3.99345, 3.87673, 3.76102, 3.63909, 3.21671,
 2.70757, 2.53961, 2.35938, 2.17081, 1.98698, 1.81773, 1.63728, 1.44259, 0.77743,
 0.64629, 0.498417, 0.369751, 0.265321, -0.209834, 0.185249, 0.131871, 0.0834604}
```



```
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```

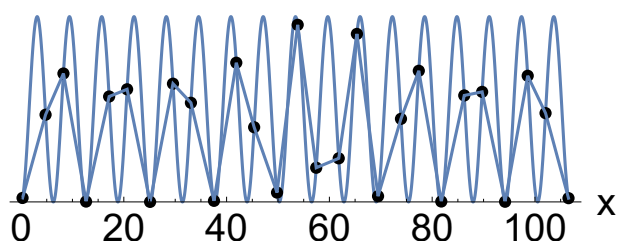
```
N = 27 a_o minimum
```

```
ENERGY 23.78875624904131
```

```
SetXX = {0.2932250554017254, 4.771056388745123, 8.25060811033398,
 12.652529235574034, 17.140502405389242, 20.63801801475526,
 25.111937817324687, 29.56505564295046, 33.05713860090859,
 37.54674330395498, 41.88456849047117, 45.358039994562795,
 49.81254862891624, 53.82945194241228, 57.43642573656314, 61.81905804716673,
 65.35337534793156, 69.46878508555494, 73.93060958605376, 77.39775269706449,
 81.77438894854795, 86.24387119582828, 89.72457146297494, 94.18743039331527,
 98.58997662718113, 102.0602649110933, 106.52969227657725`}
```

Eigenvalues

```
{4.28427, 4.25734, 4.18649, 4.10622, 4.00155, 3.88348, 3.76633,
 3.60079, 3.20622, 3.19316, 2.62094, 2.49975, 2.29923, 2.10596,
 1.90269, 1.76669, 1.48828, 1.46651, 0.749903, 0.705812, 0.511684,
 0.423109, 0.3062, 0.225402, 0.163631, 0.128297, 0.00974861}
```



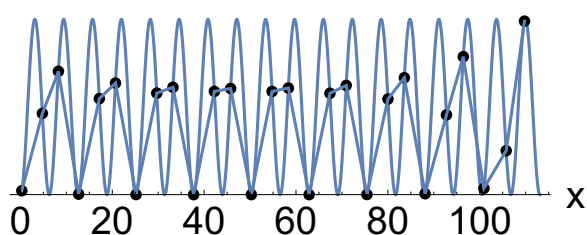
```
SP by node147 energy = 24.5574 detHess - 4953.33
```

```
node147 = {0.3011042118, 4.7860083201, 8.2736211081,
 12.6744697859, 17.1832072275, 20.6965063240,
 25.1719165928, 29.6864922060, 33.2136244605,
 37.7151248025, 42.2326374195, 45.7661034950,
 50.2769685887, 54.7993195611, 58.3375686154,
 62.8521270159, 67.3869579717, 70.9341325899,
 75.4506393366, 80.0195377361, 83.5925805874,
 88.1082528911, 92.7670901624, 96.4299843054,
 100.9117188450, 105.7650738969, 109.7514656869}
```

```
SetXX = {0.3006866933980962, 4.785653058378969, 8.273302035661809,
  12.674316855694679, 17.183068400533237, 20.696394855134727,
  25.171862867640492, 29.68644254053682, 33.213586701935114,
  37.71510744308364, 42.23262310214338, 45.76609476696376, 50.27696729393182,
  54.79932440491886, 58.33757873763226, 62.85214022503511, 67.38698747411334,
  70.93417376519898, 75.45068206459929, 80.01962468588088, 83.59270385848187,
  88.10837132335628, 92.76732096706567, 96.43034828529045,
  100.91200701244, 105.76555376658058, 109.75237651240374`}
```

Eigenvalues

```
{4.30944, 4.27497, 4.2177, 4.14063, 4.0477, 3.94415, 3.83666,
  3.73884, 3.21756, 2.78283, 2.65722, 2.48326, 2.2893, 2.08821,
  1.88808, 1.69631, 1.53009, 1.43593, 0.74912, 0.62653, 0.497566,
  -0.381151, 0.380317, 0.280911, 0.202932, 0.14913, 0.120253}
```



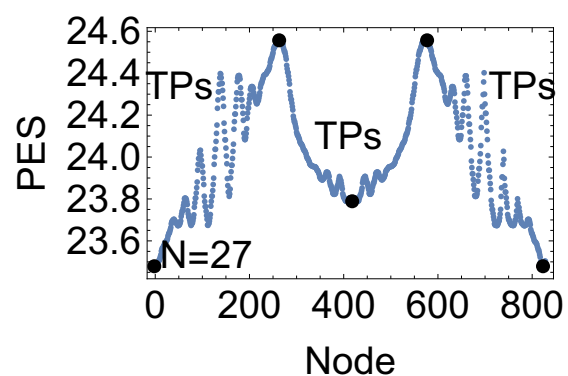
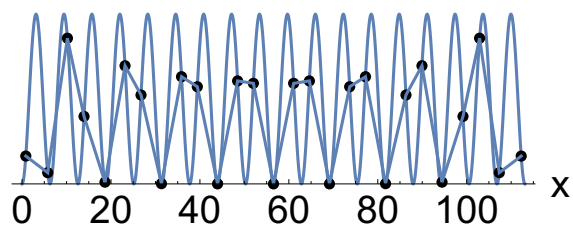
```
gMin by node405 energy = 23.48187 detHess 3330.42
node405 = {0.7805892193, 5.7243285139, 10.1378434614,
  13.8971717870, 18.6278398651, 23.1385970335,
  26.7375630151, 31.3360231238, 35.8546585320,
  39.4103917326, 43.9563663186, 48.4764114438,
  52.0200948375, 56.5470048030, 61.0722522565,
  64.6151855699, 69.1356882305, 73.6768414489,
  77.2292429194, 81.7480381185, 86.3334187643,
  89.9206044469, 94.4345312198, 99.1341382486,
  102.8488365289, 107.2972317683, 112.2101505134}
```

ENERGY 23.479140594223274

```
SetXX = {0.8339073918713161, 5.7632603318627895, 10.195798243267893,
  13.931468806811159, 18.646057999067036, 23.158550886016606,
  26.751309773478113, 31.342927785533785, 35.861611862790454,
  39.41565104214815, 43.95908851493406, 48.47931943586028, 52.022652261651096,
  56.548667764616276, 61.07468326758146, 64.61801609337228,
  69.1382470142985, 73.68168448708442, 77.23572366644211, 81.75440774369878,
  86.34602575575444, 89.93878464321595, 94.45127753016551, 99.1658667224214,
  102.90153728596466, 107.33407519736976, 112.26342813736123`}
```

Eigenvalues

```
{4.31058, 4.2762, 4.21595, 4.1328, 4.02999, 3.91278, 3.79253,  
 3.69952, 3.68376, 2.78105, 2.67024, 2.49659, 2.29676, 2.08616,  
 1.87456, 1.67465, 1.52472, 1.21307, 1.20867, 0.71106, 0.570197,  
 0.437828, 0.323006, 0.22882, 0.157135, 0.104722, 0.0971476}
```



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ==
```

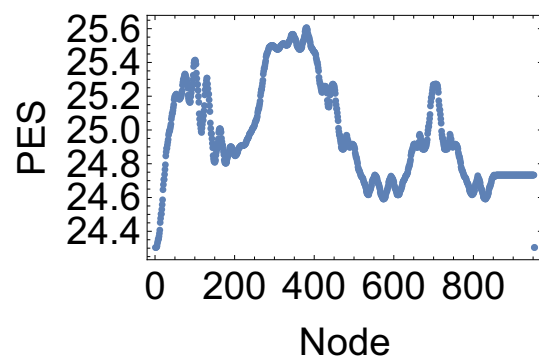
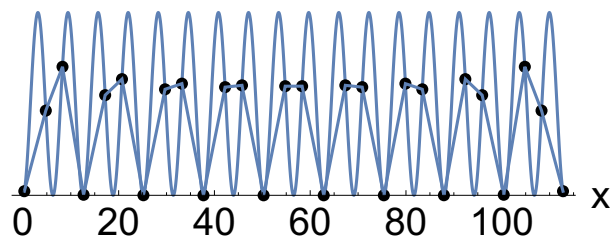
N = 28 a_o minimum

ENERGY 24.303934573538182

```
SetXX = {0.3005512102750477, 4.785388168091295, 8.27288838361323,
 12.673922777961055, 17.182302104770798, 20.695329849497533,
 25.17078887394642, 29.68428636451146, 33.21069136298118, 37.712120084040876,
 42.226556679203576, 45.75804675079936, 50.26860731777638,
 54.7822927400075, 58.31504278922506, 62.82872821145618, 67.33928877843319,
 70.87077885002897, 75.38521544519168, 79.88664416625137, 83.4130491647211,
 87.92654665528613, 92.40200567973503, 95.91503342446175, 100.4234127512715,
 104.82444714561932, 108.31194736114125, 112.7967843189575`}
```

Eigenvalues

```
{4.30702, 4.27094, 4.2133, 4.13545, 4.03994, 3.93156, 3.82001,
 3.72785, 3.2181, 3.21659, 2.73541, 2.58345, 2.39795, 2.19855,
 1.9955, 1.79701, 1.6143, 1.44959, 1.43039, 0.772984, 0.676677,
 0.556144, 0.439532, 0.336702, 0.251793, 0.186909, 0.143001, 0.119203}
```



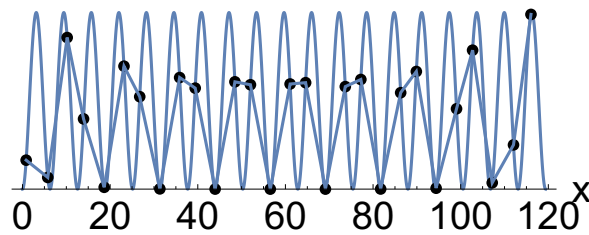
SP by node295 energy 25.50084 detHess - 4489

Setxx = node295

```
SetXX = {0.8338560130550746, 5.763174426160773, 10.195603258695328,
 13.93130459955778, 18.64589101650085, 23.15821759396586, 26.75094105421525,
 31.342541178996836, 35.860821797523094, 39.41466604332298,
 43.958051151443314, 48.47719263625636, 52.01989274410664,
 56.545783115619024, 61.068788842134765, 64.61022117220637,
 69.13018772096127, 73.66530303223986, 77.21353173143721,
 81.73201607572217, 86.30108590372333, 89.87445041810534,
 94.39088272890848, 99.04993023783439, 102.71300361946481,
 107.19501266874668, 112.0487429731388, 116.03575121418345`}
```

Eigenvalues

```
{4.31194, 4.28211, 4.22953, 4.15749, 4.06956, 3.97026, 3.86499,
 3.76275, 3.68986, 2.79578, 2.70815, 2.55602, 2.37639, 2.18475, 1.98987,
 1.79859, 1.62151, 1.50014, 1.21094, 0.720426, 0.588298, 0.461099,
 -0.381177, 0.348272, 0.253603, 0.180007, 0.130979, 0.0999559}
```



```
next node611 energy 24.6015 detHess 0.55 BBP point crossed ?
```

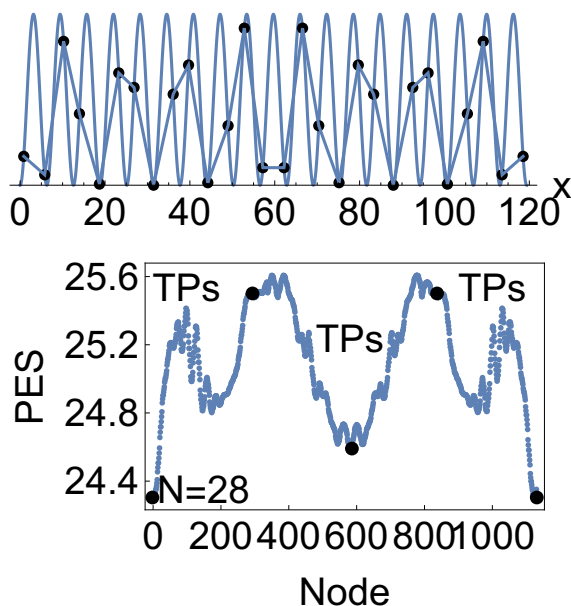
```
node611 = {0.9286729518, 5.8507387168, 10.3533439211,
14.0537346563, 18.7516227538, 23.3516696893,
26.9725005030, 31.5582461045, 36.2862083999,
40.0214529308, 44.4878984466, 49.4389029510,
53.6539533096, 57.6244928272, 62.4750628213,
66.9763634296, 70.6343573186, 75.2911406340,
79.8410365223, 83.4265905446, 87.9971270786,
92.6001929916, 96.2056591140, 100.7371897031,
105.4734866346, 109.2359983624, 113.6578451455,
118.6116213471}
```

```
ENERGY 24.59094373883594
```

```
SetXX = {0.8465280703551948, 5.784302751741412, 10.243632909131696,
13.972598994479092, 18.688054243027505, 23.24270917627786,
26.847888587892005, 31.44266752568925, 36.06418434864406,
39.68775691508881, 44.225293448227106, 49.00344196092373,
52.828878336009375, 57.20082953412003, 62.17968670331031,
66.5516342536517, 70.37707400583372, 75.15522467966629, 79.69276092805339,
83.31633430195824, 87.93785204180072, 92.53263069044279,
96.13781017017205, 100.69246576270132, 105.40792097901127,
109.13688686842814, 113.59621752204212, 118.53399239348944`}
```

Eigenvalues

```
{4.32927, 4.28681, 4.23864, 4.15718, 4.07581, 3.95184, 3.88803,
 3.71701, 3.7127, 2.90887, 2.73788, 2.59893, 2.40375, 2.21775, 1.99259,
 1.83776, 1.58366, 1.51268, 1.19328, 1.19126, 0.543449, 0.513821,
 0.333568, 0.276728, 0.173774, 0.122017, 0.105951, 0.0196797}
```



by node517 iMin energy 24.6162 detHess - 16.537338

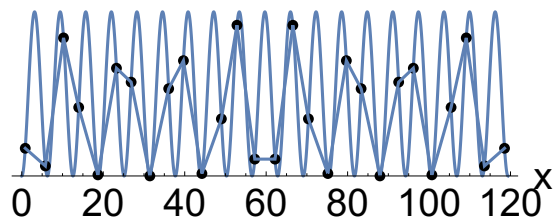
```
node517 = {0.6978950622, 5.6663789338, 10.0564298275,
13.8560020138, 18.6163070522, 23.1454724610,
26.7601162144, 31.3731598224, 35.9434497524,
39.5307787484, 44.0842735475, 48.7395680904,
52.3958696595, 56.8996435901, 61.7472318285,
65.7106935622, 69.9338945337, 74.8874605014,
79.3521832992, 83.0909889382, 87.8168273385,
92.3954359403, 96.0134178706, 100.6124780856,
105.2929612336, 108.9746745734, 113.4874798781,
118.3806071034}
```

ENERGY 24.590943738836

```
SetXX = {0.8465280311792027, 5.784302584327978, 10.243632623947072,
13.972598772479728, 18.68805412934336, 23.242709019637605,
26.847888474281724, 31.44266755216628, 36.064184450214725,
39.68775699076301, 44.22529352384282, 49.00344236980923,
52.82887904853055, 57.20082975653504, 62.17968660391095,
66.55163390602877, 70.37707387085402, 75.15522467018512,
79.69276099111428, 83.31633435755357, 87.9378520712996, 92.53263072506988,
96.13781008852179, 100.69246567502904, 105.40792080495119,
109.1368867367416, 113.59621750921937, 118.53399243435858`}
```

Eigenvalues

```
{4.32927, 4.28681, 4.23864, 4.15718, 4.07581, 3.95184, 3.88803,
 3.71701, 3.7127, 2.90887, 2.73788, 2.59893, 2.40375, 2.21775, 1.99259,
 1.83776, 1.58366, 1.51268, 1.19328, 1.19126, 0.543449, 0.513821,
 0.333568, 0.276728, 0.173774, 0.122017, 0.105951, 0.0196796}
```



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ==
```

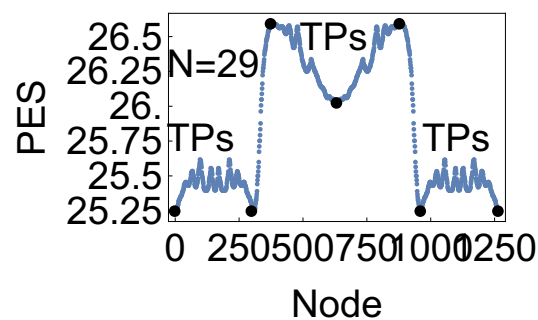
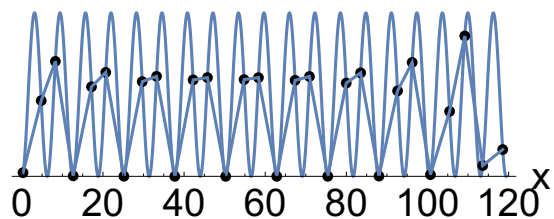
```
N = 29 a_o minimum
```

```
ENERGY 25.247194310158566
```

```
SetXX = {0.300634300571488, 4.785550623010822, 8.273142064863817,
 12.674164468262488, 17.182772094761503, 20.69598298532193,
 25.17144760738437, 29.685608943958872, 33.21246683911185,
 37.71395258570201, 42.23027853014957, 45.762980343336494,
 50.273736648831495, 54.792747051992976, 58.32884409247003,
 62.843101104603235, 67.3686059123651, 70.9094951375796, 75.42547646135347,
 79.9687071869492, 83.5219896103919, 88.03910044434579, 92.6306485086061,
 96.22326983639073, 100.73511412667422, 105.44969252975602,
 109.18548332747011, 113.61759567276421, 118.54681389663266`}
```

Eigenvalues

```
{4.31, 4.27826, 4.22524, 4.15264, 4.06273, 3.9592, 3.84911,
 3.74846, 3.68856, 3.21748, 2.76741, 2.64535, 2.47809, 2.291, 2.09578,
 1.90027, 1.71323, 1.55388, 1.43752, 1.21123, 0.755633, 0.642816,
 0.520378, 0.406923, 0.308523, 0.227954, 0.166998, 0.127335, 0.0998203}
```




```

by node309 mirror gMin energy = 25.24723 detHess 11 250.39
0.8407029842 × 5.7678728111 × 10.2022358498
13.9351289420 × 18.6476816962 × 23.1597286036
26.7515798433 × 31.3422772755 × 35.8593920107
39.4124492727 × 43.9553647410 × 48.4713510559
52.0121731593 × 56.5375656899 × 61.0518563738
64.5879497643 × 69.1069241101 × 73.6177842760
77.1505391843 × 81.6668646741 × 86.1686463573
89.6956677695 × 94.2098722735 × 98.6861785211
102.1997858169 × 106.7085925499 × 111.1120375296
114.6001653819 × 119.0859844075

```

```

SP node384 energy = 26.59247 detHess - 1730.68
node384 = {3.9036915673, 7.4038838695, 11.8044807455,
15.5147875625, 19.4170708731, 23.8568924036,
27.3398965298, 31.6271654963, 36.1241059440,
39.6210552519, 44.0569833228, 48.5675281521,
52.0861466696, 56.5737102860, 61.0863138064,
64.6141460640, 69.1196961463, 73.6299039791,
77.1595562119, 81.6711112727, 86.1723687948,
89.6980417533, 94.2105161537, 98.6857357234,
102.1983762463, 106.7063531690, 111.1067416882,
114.5939587200, 119.0784261858}
Setxx = node384

```

```

SetXX = {3.9003412137011493, 7.4011176012978845, 11.801091644408874,
15.508327471906751, 19.41387567290484, 23.854265035838093,
27.337076549241335, 31.62582553565011, 36.12293563947713,
39.620060214806465, 44.05650535625081, 48.56709061343294,
52.08580514051032, 56.57354916194375, 61.08617201350525, 64.6140482635192,
69.11966286419293, 73.62990193360108, 77.15958580438723, 81.67116689837115,
86.17250607645751, 89.69823054977292, 94.21072587464816,
98.68617594489609, 102.19892776122279, 106.70696262423465,
111.10801502117387, 114.5953776918751, 119.08009494557095` }

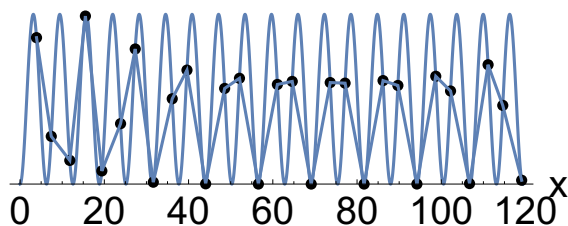
```

Eigenvalues

```

{4.30484, 4.26665, 4.21047, 4.13835, 4.05158, 3.95244, 3.84649,
3.74668, 3.63885, 3.21715, 2.72848, 2.58406, 2.42423, 2.25639, 2.08521,
1.92444, 1.76998, 1.60655, 1.44038, 0.783186, 0.676087, 0.544014,
0.42242, 0.318819, 0.234447, -0.209971, 0.169787, 0.127361, 0.0833444}

```



```
iMin node944 energy = 26.024087 detHess 126.247919
node944 = {6.5304659691 × 10.9662500122 × 14.4024639811 ×
18.8036926108 × 23.1590740065 × 26.5945161817 ×
31.0240214108 × 35.0715768484 × 38.6274177681 ×
42.9838647032 × 46.4996886396 × 50.5999618359 ×
55.0285124773 × 58.4583451021 × 62.8313049707 ×
67.2037167381 × 70.6335491555 × 75.0620149949 ×
79.1605704044 × 82.6774771016 × 87.0337238745 ×
90.5878306400 × 94.6373904506 × 99.0667787127 ×
102.5018444536 × 106.8579387811 × 111.2578076754 ×
114.6935681072 × 119.1290050549},
```

```
iMin by node632 energy = 26.024122 Peak by 800 is TP not SP
```

```
node631 = {6.5264062535, 10.9625138842, 14.3991679602,
18.8016956569, 23.1563813584, 26.5921868554,
31.0217992661, 35.0674091614, 38.6249378392,
42.9815841207, 46.4963743799, 50.5982999748,
55.0269327992, 58.4567688909, 62.8302550374,
67.2021431501, 70.6319786302, 75.0603642223,
79.1572814852, 82.6752285156, 87.0312911543,
90.5837634958, 94.6352176376, 99.0644893599,
102.4991975610, 106.8559620724, 111.2545262525,
114.6898584055, 119.1249545462}
```

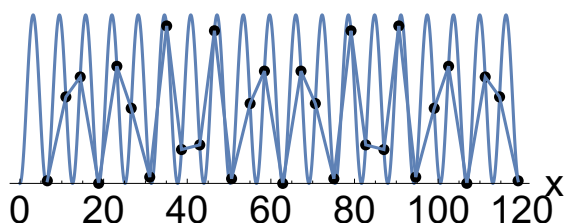
```
Setxx = node631
```

```
ENERGY 26.0240823560639
```

```
SetXX = {6.53258414264245, 10.968195786225786, 14.404182197566078,
18.80473133606861, 23.160470898177284, 26.59572447075907, 31.02517184010053,
35.07373287767578, 38.62870316523851, 42.98504900524955, 46.50141387827811,
50.60082723133376, 55.0293353427395, 58.45916742864535, 62.83185307179587,
67.2045387149464, 70.63437080085225, 75.06287891225799, 79.16229226531365,
82.6786571383422, 87.03500297835323, 90.58997326591599, 94.63853430349123,
99.06798167283267, 102.50323524541446, 106.85897480752313,
111.25952394602567, 114.69551035736595, 119.13112200094929`}
```

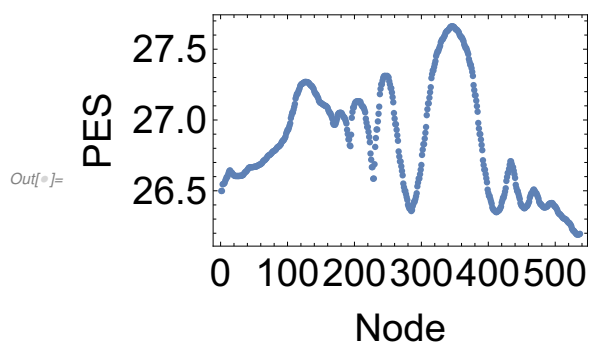
Eigenvalues

```
{4.2772, 4.23994, 4.20126, 4.12045, 4.0233, 3.92198, 3.80698,
3.65032, 3.56013, 3.14561, 3.14419, 2.58305, 2.43703, 2.29441, 2.1142,
1.96309, 1.79027, 1.55211, 1.54785, 0.790152, 0.655023, 0.629098,
0.448315, 0.324967, 0.269394, 0.194091, 0.148601, 0.0301811, 0.0157053}
```



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

```
new N = 30 search minimum
```



```
ende near mirror gMin?
```

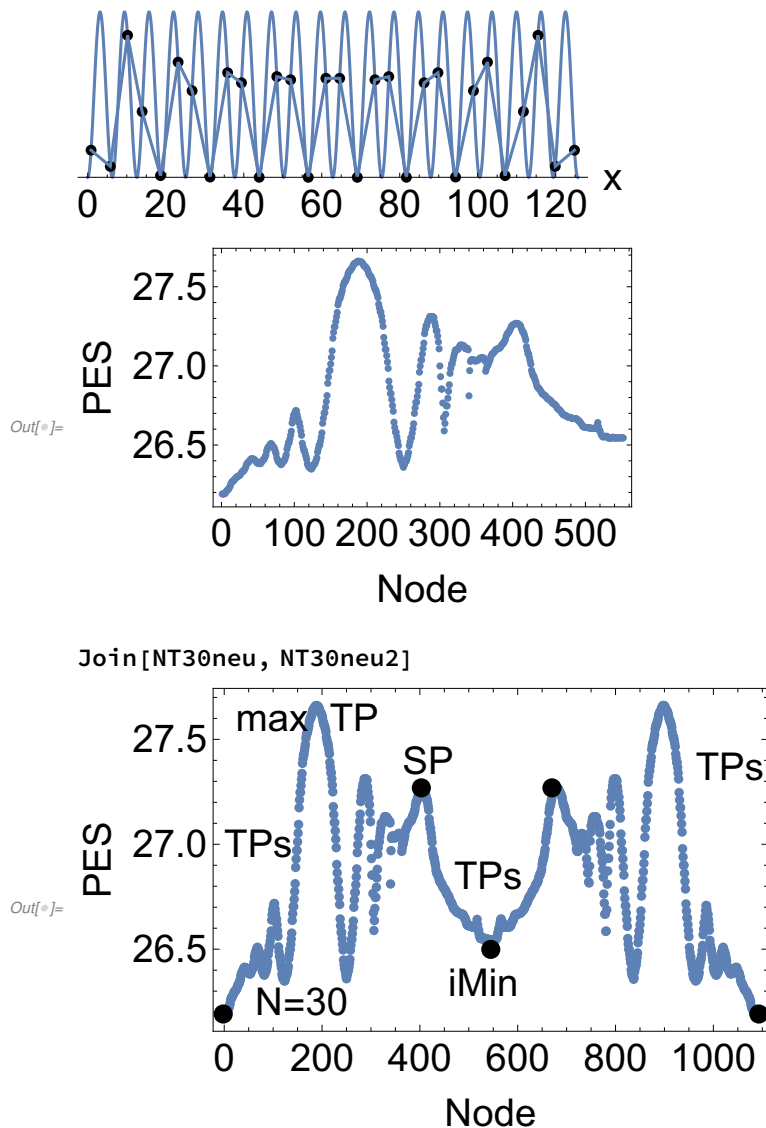
```
node1298 = {0.8805101643, 5.7954560171, 10.2417806887,
13.9590073900, 18.6604057491, 23.1737798027,
26.7615485977, 31.3476352814, 35.8654837780,
39.4176740977, 43.9589668833, 48.4769315182,
52.0185110759, 56.5435324451, 61.0634185163,
64.6027707155, 69.1221670979, 73.6486921465,
77.1911442324, 81.7090451515, 86.2545788800,
89.8097836790, 94.3276010309, 98.9251556180,
102.5233189249, 107.0339370423, 111.7625767614,
115.5189439732, 119.9346841507, 124.8766563994}
Setxx = node1298
```

```
ENERGY 26.19053397195808
```

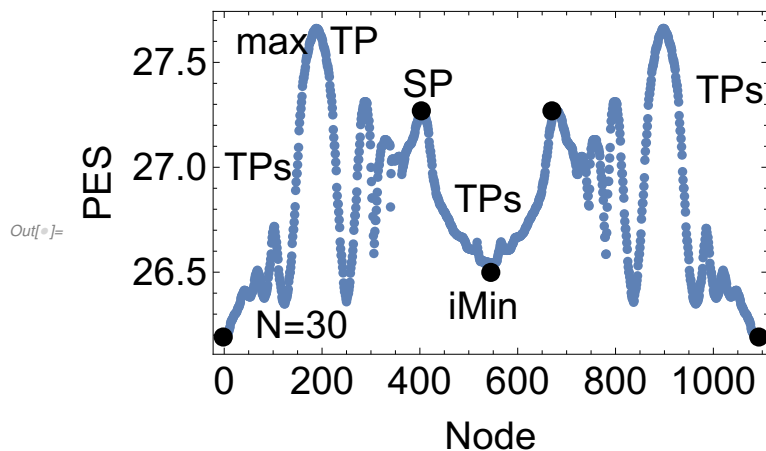
```
SetXX = {0.8337984498248611, 5.763078177757982, 10.195384801732041,
13.931120657681603, 18.645703973341146, 23.157844275729996,
26.750528182567127, 31.342108233031748, 35.859937003433835,
39.413563643044995, 43.95688956802742, 48.47481064431587, 52.01680710626661,
56.54255253843404, 61.062182782533306, 64.60152336105843,
69.12115360515769, 73.64689903732513, 77.18889549927587, 81.70681657556432,
86.25014250054674, 89.80376914015791, 94.32159791055999, 98.9131779610246,
102.50586186786173, 107.01800217025058, 111.73258548591012,
115.46832134185968, 119.90062796583373, 124.8299076937668}
```

Eigenvalues

```
{4.31228, 4.28476, 4.23611, 4.16841, 4.08379, 3.98525, 3.87801, 3.77321,
 3.6966, 3.68412, 2.78506, 2.69524, 2.54843, 2.37517, 2.18951, 1.99952,
 1.81238, 1.64009, 1.51732, 1.21229, 1.20983, 0.730345, 0.606964,
 0.485301, 0.375611, 0.281429, 0.204558, 0.146474, 0.102987, 0.097829}
```



```
Join[NT30neu, NT30neu2]
```

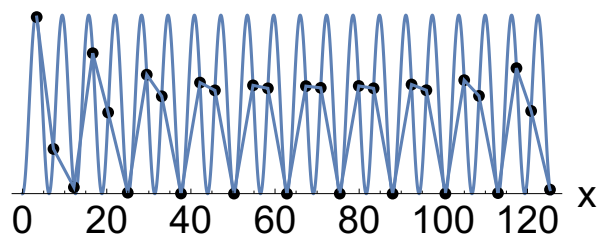


```
sp by former node406 energy = 27.2688 detHess - 6201.08
nodesp = {3.3707709542, 7.3454275385, 12.1935335757,
16.6773805911, 20.3366714201, 24.9924630512,
29.5084361172, 33.0805571937, 37.6482790587,
42.1651900282, 45.7122824477, 50.2467310377,
54.7624293068, 58.3012456047, 62.8235850907,
67.3376566899, 70.8729912624, 75.3908631091,
79.9013744453, 83.4336963501, 87.9495939158,
92.4504916594, 95.9769291704, 100.4908549856,
104.9646816254, 108.4770867485, 112.9852499657,
117.3815621637, 120.8681440829, 125.3512691150}
Setxx = nodesp
```

```
SetXX = {3.3449177858616466, 7.3317809131454625, 12.185367625022712,
  16.6671026134872, 20.330139939522947, 24.989110894116646,
  29.504944846109424, 33.07808596493549, 37.6470563778958, 42.1639948322249,
  45.7114068511954, 50.246313459435086, 54.76205224359453, 58.30098973432338,
  62.823496637756215, 67.33764720440402, 70.87306269016688,
  75.39100215728779, 79.901720158309, 83.43417697682594, 87.95012259119122,
  92.45159700136412, 95.97836355861314, 100.49239121231744,
  104.96785472858576, 108.48102871430359, 112.98959035874486,
  117.39061518106382, 120.87818824470062, 125.36308858040485`}
```

Eigenvalues

```
{4.31139, 4.28346, 4.23664, 4.17294, 4.09485, 4.0058, 3.9101, 3.81367,
  3.72984, 3.21745, 2.78775, 2.68471, 2.5358, 2.36598, 2.18683, 2.00547,
  1.82739, 1.65924, 1.51909, 1.43672, 0.760004, 0.655108, 0.538604,
  0.428496, -0.381156, 0.331017, 0.249391, 0.185943, 0.142436, 0.118921}
```



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ==
```

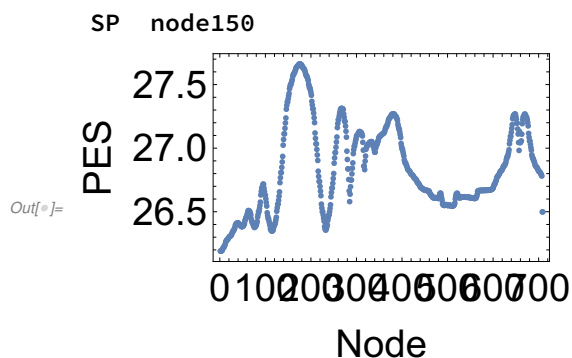
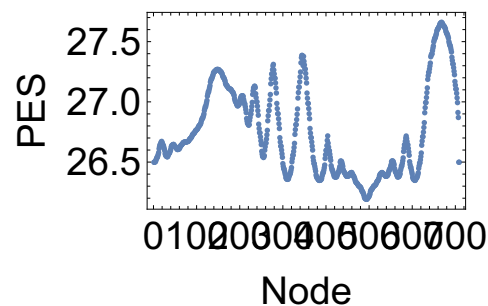
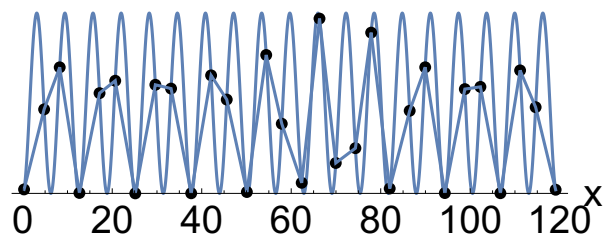
```
N = 30 a_o minimum
```

```
ENERGY 26.498606010646828
```

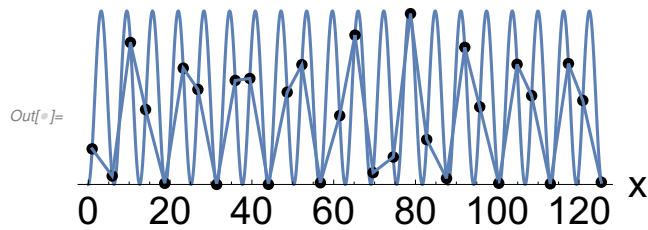
```
SetXX = {0.2977112072266914, 4.779834196219048, 8.26423064851429,  
12.665648805548162, 17.16618189167979, 20.67304508419971,  
25.148150753907153, 29.638665138989534, 33.15041802721074,  
37.64880254601983, 42.09689898890968, 45.59407562212389, 50.09041283036267,  
54.412573288042836, 57.89030474091205, 62.341894055438814,  
66.32289354893662, 69.96151389305926, 74.3490837189982, 77.869658246974,  
82.01134259365386, 86.47700708165891, 89.94613143201377, 94.3320809660334,  
98.8022321696619, 102.28482962509712, 106.75071677461801,  
111.15321305021595, 114.62458980131572, 119.09501893953679`}
```

```
Eigenvalues
```

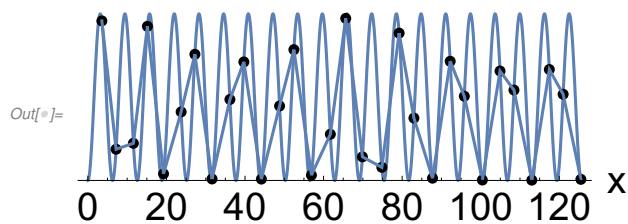
```
{4.29141, 4.26512, 4.21274, 4.14188, 4.06026, 3.95819, 3.85261, 3.74983,  
3.59964, 3.21293, 3.19475, 2.65657, 2.53859, 2.37799, 2.19932, 2.01936,  
1.8558, 1.71743, 1.48552, 1.45338, 0.763715, 0.714166, 0.565397,  
0.448146, 0.367758, 0.264453, 0.207184, 0.151743, 0.125454, 0.00573032}
```



TP peak 26.35048 node114 energy = 26.3504814 detHess - 214.9 gradNorm 0.13966
node114 = {0.9401582063, 5.8378425547, 10.3047593187,
14.0009483325, 18.6878744911, 23.2138226925,
26.7997558086, 31.3810636543, 35.9275156787,
39.4940602857, 44.0355878953, 48.6303810321,
52.2272409507, 56.7486438374, 61.4686926226,
65.2102201601, 69.6430040260, 74.5795650753,
78.7858957416, 82.7486226335, 87.5872092629,
92.0573050515, 95.7133352710, 100.3638329254,
104.8479755820, 108.4092672270, 112.9702632866,
117.4045287897, 120.9197685076, 125.4345118676}
SetXX = node114



summit TP at node176 energy = 27.661343 detHess 4.012626 gradNorm 0.2311
node176 = {3.5553313744, 7.1786719300, 11.5825262991,
15.1537476691, 19.2512460553, 23.7397190372,
27.2439520945, 31.6056807803, 36.1560270303,
39.7067571803, 44.1635766648, 48.8006844204,
52.4434047190, 56.9074161298, 61.7225301014,
65.6422466190, 69.8871403612, 74.8296768512,
79.2338052777, 82.9983251296, 87.7307901419,
92.2315753078, 95.8299254985, 100.4282112849,
104.9239241629, 108.4702223697, 113.0128868311,
117.4712029303, 120.9862721756, 125.5007308396}
SetXX = node176



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ==
```

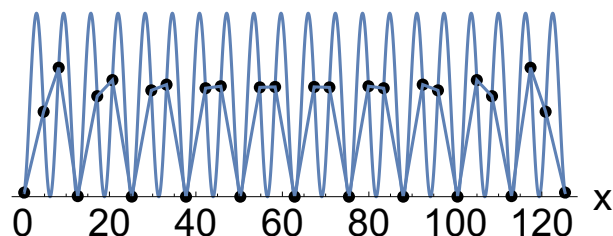
```
N = 31 a_o minimum
```

```
ENERGY 27.015385207340543
```

```
SetXX = {0.30056925351095193, 4.7854234456989, 8.272943469163254,
12.673975263360376, 17.182404172001785, 20.695471673855465,
25.170931936839544, 29.68457362490505, 33.21107685650118, 37.71251811984508,
42.227365258379024, 45.75911750374454, 50.26972176212389, 54.78456531249253,
58.31803438465911, 62.83185307179586, 67.34567175893262, 70.87914083109919,
75.39398438146783, 79.90458863984718, 83.4363408852127, 87.95118802374665,
92.45262928709055, 95.97913251868668, 100.49277420675217,
104.96823446973626, 108.48130197158994, 112.98973088023135,
117.39076267442847, 120.87828269789283, 125.36313689008077`}
```

```
Eigenvalues
```

```
{4.30946, 4.27997, 4.23274, 4.16866, 4.08926, 3.99721, 3.89726, 3.79873,
3.72129, 3.21773, 3.21702, 2.74942, 2.62208, 2.4617, 2.28596, 2.104,
1.92222, 1.74713, 1.58917, 1.44608, 1.43213, 0.778242, 0.696974, 0.589962,
0.482097, 0.383226, 0.297614, 0.227477, 0.174078, 0.137918, 0.118106}
```



```
SP node351 iMin node698 node722 node747 SP node1091 node1430
```

```
SP node351 energy = 28.2118107 detHess - 13455.57
```

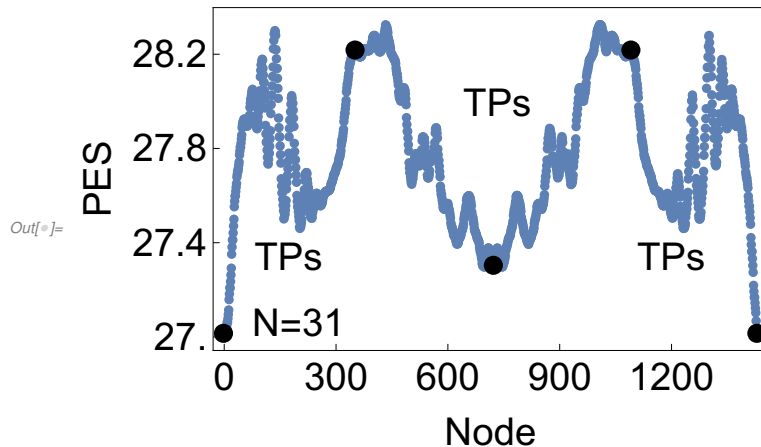
```
0.8439709853 × 5.7702390541 × 10.2057606724
13.9373045882 × 18.6489424188 × 23.1613096825
26.7528635041 × 31.3432010477 × 35.8608771937
39.4141023263 × 43.9569494819 × 48.4744516833
52.0161076255 × 56.5416378886 × 61.0601383336
64.5987550743 × 69.1182046419 × 73.6408204671
77.1807968929 × 81.6984322814 × 86.2330901357
89.7806337254 × 94.2982556465 × 98.8663321750
102.4388081102 × 106.9550194298 × 111.6116345146
115.2718680212 × 119.7553217897 × 124.6048628655
128.5826145316
```

```
iMin node698
```

```
node722 energy = 27.3040639 detHess - 523.289
```

```
0.8435823362 × 5.777301732 × 10.2276722983
13.9582448357 × 18.6728534692 × 23.2116777684
26.8112209877 × 31.4049719466 × 35.9877685353
39.5804256034 × 44.1252582663 × 48.8125655723
52.5068126181 × 56.9845497147 × 61.8844968629
65.9725691958 × 70.0615180582 × 74.9618296783
79.4394671230 × 83.1339947824 × 87.8215437084
92.3665294287 × 95.9593201287 × 100.5422227036
```


105.1363828294 \times 108.7362589059 \times 113.2750568822
 117.9906421365 \times 121.7225483946 \times 126.1715076748
 131.1067243221
 node747 SP 1091 energy = 28.21781696 detHess - 14 748.81
 3.3453144887 \times 7.3320241273 \times 12.1855786374
 16.6674773135 \times 20.3304632226 \times 24.9894118328
 29.5055212867 \times 33.0787457278 \times 37.6477390522
 42.1653821795 \times 45.7131599230 \times 50.2481543616
 54.7658215715 \times 58.3058872362 \times 62.8286263736
 67.3481388184 \times 70.8868179605 \times 75.4053678641
 79.9310618849 \times 83.4728318888 \times 87.9903624146
 92.5336582030 \times 96.0872074600 \times 100.6048917260
 105.1964354844 \times 108.7890797095 \times 113.3011675374
 118.0156788513 \times 121.7513238992 \times 126.1836708243
 131.1128672362
 node1430 energy = 27.015436
 6.5769406041 \times 11.0628035263 \times 14.5509254827
 18.9546635979 \times 23.4633159645 \times 26.9768282233
 31.4532284374 \times 35.9669219031 \times 39.4936110719
 43.9953829186 \times 48.5102401601 \times 52.0420593900
 56.5527804005 \times 61.0676140352 \times 64.6010994394
 69.1149581734 \times 73.6287367018 \times 77.1621893664
 81.6770427745 \times 86.1875299777 \times 89.7192151057
 94.2340520382 \times 98.7351618325 \times 102.2614790269
 106.7750684273 \times 111.2495859811 \times 114.7622105641
 119.2704130085 \times 123.6687299764 \times 127.1556703490
 131.6395050787



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ==
```

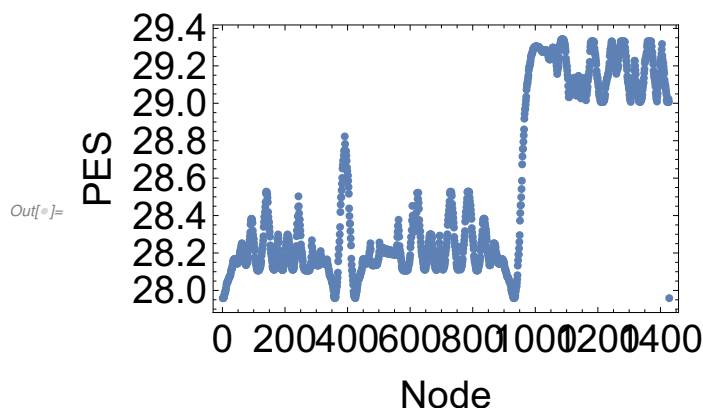
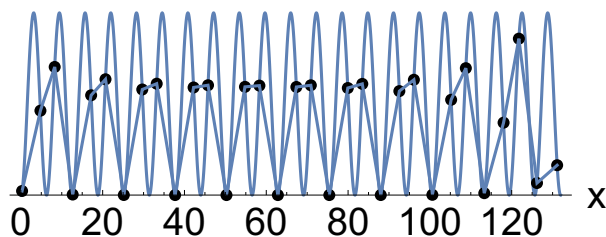
```
N = 32 a_o minimum
```

```
ENERGY 27.958662314733377
```

```
SetXX = {0.300598885681983, 4.785481381444698, 8.273033937703183,
12.674061457241635, 17.182571786178734, 20.69570459675505,
25.17116686608475, 29.685045317380407, 33.2117100136547, 37.71317168361962,
42.22869273090841, 45.76087669535043, 50.271551281149414,
54.788294653408094, 58.322953950467934, 62.83698053064666,
67.3561345472087, 70.89292867288898, 75.40835537401829, 79.93391358967357,
83.47504251077494, 87.99144579517824, 92.53469734769492,
96.08805447714137, 100.60532146098161, 105.19687649160137,
108.78951140233363, 113.3014200790992, 118.01599954908629,
121.75177838648919, 126.18393299781613, 131.11316460264663`}
```

```
Eigenvalues
```

```
{4.31177, 4.28583, 4.24226, 4.18228, 4.10738, 4.01975, 3.92307, 3.82426, 3.73803,
3.68816, 3.21742, 2.77431, 2.67311, 2.52935, 2.36516, 2.19122, 2.01411,
1.83956, 1.67549, 1.54032, 1.43764, 1.2112, 0.764786, 0.668053, 0.557524,
0.451309, 0.355779, 0.273819, 0.207093, 0.156859, 0.124375, 0.099823}
```



```
start
```

```
0.300598885681983, 4.785481381444698, 8.273033937703183, 12.674061457241635,
17.182571786178734, 20.69570459675505, 25.17116686608475,
29.685045317380407, 33.2117100136547, 37.71317168361962, 42.22869273090841,
45.76087669535043, 50.271551281149414, 54.788294653408094,
58.322953950467934, 62.83698053064666, 67.3561345472087, 70.89292867288898,
75.40835537401829, 79.93391358967357, 83.47504251077494, 87.99144579517824,
92.53469734769492, 96.08805447714137, 100.60532146098161, 105.19687649160137,
108.78951140233363, 113.3014200790992, 118.01599954908629,
121.75177838648919, 126.18393299781613, 131.11316460264663`
```

```
SP ? node114
```

nodes 166 × 193 × 226 × 267

gMin node361 energy = 28.09515294 detHess 10 695.93

0.8394414333 × 5.7670019354 × 10.2009980537

13.9344069576 × 18.6473303831 × 23.1594037958

26.7514087405 × 31.3422680789 × 35.8595355486

39.4127074184 × 43.9557007895 × 48.4721009352

52.0131710582 × 56.5386364971 × 61.0540708366

64.5908503878 × 69.1099723439 × 73.6240282867

77.1586986035 × 81.6754338058 × 86.1861938560

89.7184263537 × 94.2339545268 × 98.7356580594

102.2624583976 × 106.7763747096 × 111.2525244927

114.7659819928 × 119.2746559869 × 123.6776627649

127.1656528592 × 131.6512737552

node425 again gMin energy = 28.065227035 detHess 10 050.25

0.8553562708 × 5.7781381260 × 10.2170712496

13.9440388495 × 18.6524151132 × 23.1649250526

26.7552175644 × 31.3441749618 × 35.8614423355

39.4141095046 × 43.9563976650 × 48.4727892357

52.0136990712 × 56.5389111702 × 61.0543668295

64.5911069134 × 69.1101413762 × 73.6242788557

77.1589801252 × 81.6756931622 × 86.1866903992

89.7190578588 × 94.2346058541 × 98.7369804768

102.2641583488 × 106.7781787654 × 111.2562354825

114.7706023592 × 119.2797237263 × 123.6882185807

127.1774894229 × 131.6651354616

quasi back ? like node 361

SP / iMin nodes 580 × 648 × 685 × 706 × 754 × 763 × 816

node933 gMin energy = 28.00947663 detHess 69 714.67

0.3089883016 × 4.7926148423 × 8.2794577519

12.6771429778 × 17.1853741671 × 20.6979626076

25.1722641324 × 29.6860782721 × 33.2125145285

37.7135679608 × 42.2290770074 × 45.7611791855

50.2717095391 × 54.7884669342 × 58.3231078035

62.8370848524 × 67.3562936580 × 70.8931128315

75.4085266977 × 79.9342433931 × 83.4754728743

87.9918815192 × 92.5355739967 × 96.0892481171

100.6065136239 × 105.1992559932 × 108.7929705174

113.3045917380 × 118.0219885644 × 121.7618289469

126.1907969938 × 131.1227862112

noch weiter zurueck zu start !

SP node1004 energy = 29.353187249 detHess - 10 219.87

0.3031870252 × 4.7876007942 × 8.2748416387

12.6748204100 × 17.1830365157 × 20.6958305782

25.1709198391 × 29.6841784363 × 33.2103618319

37.7116420863 × 42.2254522560 × 45.7565195958

50.2669670979 × 54.7788992398 × 58.3105611289

62.8240194770 × 67.3296443103 × 70.8582070077

75.3719503474 × 79.8594233711 × 83.3782788945

87.8891976659 × 92.3247912162 × 95.8217659642

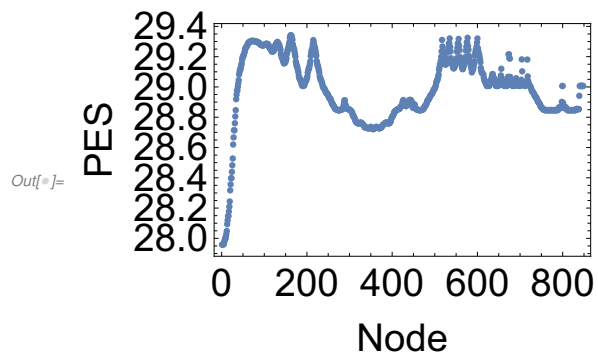
100.3187356241 × 104.6050655885 × 108.0882787552

112.5278078397 × 116.4281025742 × 120.1403492292

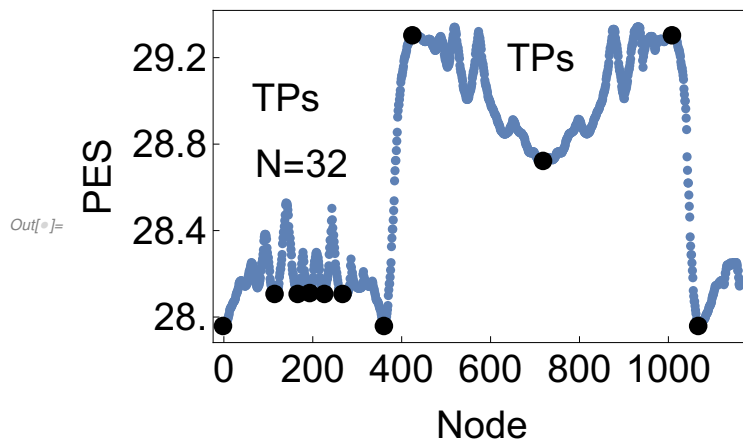
124.5413929321 × 128.0413307762

real compressed state like correct SP, but back :

o.k. is true result



SP node74 energy = 29.303485 detHess - 4642.49
 0.3057162928 \times 4.7897508247 \times 8.2767762920
 12.6757475844 \times 17.1838778919 \times 20.6965060922
 25.1712455269 \times 29.6844797461 \times 33.2105905213
 37.7117474112 \times 42.2255395330 \times 45.7565726844
 50.2669752714 \times 54.7788706718 \times 58.3105014666
 62.8239400505 \times 67.3294656958 \times 70.8579672576
 75.3716905552 \times 79.8588838351 \times 83.3775938608
 87.8884530376 \times 92.3232445016 \times 95.8199518345
 100.3166582208 \times 104.6006945736 \times 108.0842261376
 112.5228810467 \times 116.4181590402 \times 120.1351642292
 124.5371983365 \times 128.0363157445
 iMin 357 energy = 28.7380062 detHess 87.28
 0.2544885779 \times 4.6984061322 \times 8.1424214448
 12.5451256061 \times 16.9265863572 \times 20.3694218116
 24.8109605916 \times 28.9362430667 \times 32.4469015673
 36.8153606141 \times 40.4106961105 \times 44.4229100321
 48.8616178447 \times 52.3142264306 \times 56.6547758047
 61.1012342208 \times 64.5604370939 \times 69.0072172946
 73.3463851998 \times 76.7990399115 \times 81.2372827563
 85.2458565527 \times 88.8440647785 \times 93.2126743895
 96.7213679322 \times 100.8494819763 \times 105.2907545777
 108.7331503812 \times 113.1155332839 \times 117.5161129368
 120.9594876987 \times 125.4028290819



Cape eps = 5.10^{-9}
 114 energy = 28.106837097 detHess - 305.09
 166 energy = 28.1109429 detHess - 1480.4
 193 energy = 28.1097600867 detHess 1603.7
 226 energy = 28.1108199 detHess - 1731.20
 267 energy = 28.115669 detHess 188.4

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

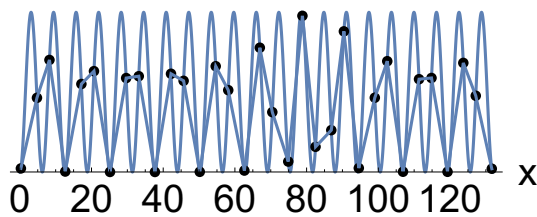
```
N = 33 a_o minimum
```

```
ENERGY 29.20944526852323
```

```
SetXX = {0.2994902597375053, 4.783313645944081, 8.269651239215383,
12.670834909472747, 17.17629277195417, 20.686995667365082,
25.162359557514858, 29.667337225350934, 33.18807845662095,
37.68861615951625, 42.17865810683542, 45.69568573804453, 50.20256429291589,
54.64656599739076, 58.14494931613436, 62.643007944398185,
66.95334168287094, 70.4332360911535, 74.88139665588695, 78.8354328874625,
82.49813916492175, 86.88975651900249, 90.40186056682656, 94.56148525222049,
99.02969554760152, 102.50032165002058, 106.89256848379421,
111.36315326136217, 114.84705585807066, 119.31499419267139,
123.71745282201981, 127.18957130487398, 131.66068065687432`}
```

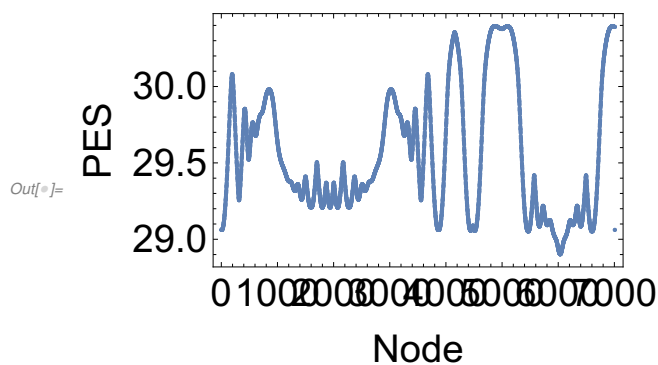
```
Eigenvalues
```

```
{4.29742, 4.27, 4.23297, 4.16935, 4.10297, 4.01753, 3.92348, 3.82759, 3.73798,
3.5994, 3.21567, 3.1958, 2.6874, 2.5652, 2.44256, 2.27445, 2.11839, 1.94725,
1.82266, 1.67252, 1.48382, 1.44625, 0.773641, 0.718812, 0.610746, 0.473857,
0.416291, 0.311837, 0.243141, 0.18923, 0.144792, 0.123257, 0.00260954}
```



ist iMin and asymmetric thus there must exist a mirror!

```
NT33 predictor 0.015
```



here emerge three minimums PP direction

because iMin is asym here is a zone of reortierung in iMin - well
start energy 29.0614251477 detHess - 141.02786319

```
0.3086734224 × 4.7948162275 × 8.2843542351 × 12.6827026028
17.1971207470 × 20.7148694915 × 25.1895606235 × 29.7210405821
33.2602097841 × 37.7622139538 × 42.3272783651 × 45.8958873916
50.4063156708 × 55.0571120774 × 58.7110463811 × 63.1950399997
68.0342886933 × 71.9912264798 × 76.2104639439 × 81.1555314176
85.5986266925 × 89.3415594831 × 94.0657657581 × 98.6089615108
102.2131991391 × 106.8112339879 × 111.4063526067 × 115.0086849447
```

119.5535873562 × 124.2706936316 × 128.0035618680 × 132.4549952427
137.3929500826

SP node853 energy = 29.9803768 detHess - 39 889.007

0.3061993997 × 4.7902465928 × 8.2773027024

12.6761010434 × 17.1844103970 × 20.6971613483

25.1718491933 × 29.6856351458 × 33.2121105506

37.7132961174 × 42.2286655109 × 45.7607004507

50.2712646938 × 54.7876111506 × 58.3219999046

62.8359514574 × 67.3540013916 × 70.8900884067

75.4053949867 × 79.9278728283 × 83.4669968152

87.9831493413 × 92.5178559387 × 96.0651905027

100.5822794543 × 105.1506607816 × 108.7233255164

113.2393021441 × 117.8967703031 × 121.5580145621

126.0408117926 × 130.8918431325 × 134.8729487401

compressed at the End

iMin1 node1594 energy = 29.20947013 detHess 396.2208

0.2947748162 × 4.7792867476 × 8.2660293285

12.6690782364 × 17.1746545615 × 20.6856421409

25.1616485563 × 29.6665583274 × 33.1873678540

37.6881173621 × 42.1778725909 × 45.6947935094

50.2016932092 × 54.6448468240 × 58.1429415342

62.6407617926 × 66.9486514716 × 70.4287237018

74.8759255019 × 78.8242540685 × 82.4919636271

86.8843426988 × 90.3946453953 × 94.5579514257

99.0264799316 × 102.4972061606 × 106.8907578713

111.3608426120 × 114.8446235164 × 119.3128713934

123.7135211257 × 127.1852795138 × 131.6558376798

further compressed

and node1606 energy = 29.20948999 detHess - 582.049

0.3049014884 × 4.7877828569 × 8.2734878149

12.6724940938 × 17.1774253496 × 20.6874810782

25.1620737713 × 29.6659948788 × 33.1859150983

37.6860645318 × 42.1731669940 × 45.6885346645

50.1947463303 × 54.6302806998 × 58.1256168432

62.6209366551 × 66.9068998883 × 70.3891807776

74.8277862626 × 78.7263902094 × 82.4395006585

86.8401505524 × 90.3387710538 × 94.5316696029

99.0046611589 × 102.4786408750 × 106.8824383154

111.3544712183 × 114.8412699538 × 119.3131177447

123.7176128963 × 127.1917079042 × 131.6648898423

and node1800 energy = 29.206646563 detHess 1816.42

0.2939625419 × 4.7770546695 × 8.2622344446

12.6652332192 × 17.1669338711 × 20.6748781939

25.1506074764 × 29.6442020873 × 33.1579131843

37.6570086279 × 42.1140132272 × 45.6149405692

50.1139573049 × 54.4620278735 × 57.9402208535

62.4023936916 × 66.4481869502 × 70.0368719004

74.4222694128 × 77.9794294829 × 82.0681034797

86.5339073803 × 90.0095094827 × 94.3748071744

98.8667914590 \times 102.3631313719 \times 106.8255081273
 111.2992425873 \times 114.7986977472 \times 119.2896427668
 123.6898344766 \times 127.1701658662 \times 131.6484433653
 and node1938 energy = 29.20772135 detHess - 1481.46
 0.2999261413 \times 4.7804302987 \times 8.2632414041
 12.6634775735 \times 17.1606686242 \times 20.6648198616
 25.1392415454 \times 29.6201635145 \times 33.1262808427
 37.6226788473 \times 42.0427180378 \times 45.5299867979
 50.0169928103 \times 54.2580574636 \times 57.7471872935
 62.1678268412 \times 65.9721677461 \times 69.7777867731
 74.1987014496 \times 77.6877418085 \times 81.9294367530
 86.4166263787 \times 89.9040713289 \times 94.3243224226
 98.8210420021 \times 102.3274218581 \times 106.8084485506
 111.2837735531 \times 114.7884210211 \times 119.2858429509
 123.6887279227 \times 127.1721883257 \times 131.6537137267
 and node2075 energy = 29.206716448 detHess 1824.28
 0.2853498313 \times 4.7655251362 \times 8.2471103300
 12.6524160004 \times 17.1436611895 \times 20.6440157550
 25.1194643266 \times 29.5816363579 \times 33.0783209419
 37.5708147622 \times 41.9353630233 \times 45.4111389060
 49.8768567625 \times 53.9636575250 \times 57.5221707422
 61.9075451681 \times 65.4947153854 \times 69.5425382252
 74.0049591168 \times 77.4830963714 \times 81.8319816138
 86.3308717278 \times 89.8317391376 \times 94.2890164487
 98.7875190528 \times 102.3008875622 \times 106.7944958661
 111.2684509795 \times 114.7755263241 \times 119.2768420691
 123.6746644476 \times 127.1586811199 \times 131.6398368926
 and node2270 energy = 29.20946757 detHess - 420.45
 0.2904898302 \times 4.7621897573 \times 8.2351161000
 12.6363078294 \times 17.1073803558 \times 20.5930957678
 25.0639336579 \times 29.4660180495 \times 32.9391066879
 37.4110635972 \times 41.5989387888 \times 45.0991732910
 49.4981434128 \times 53.2028908420 \times 57.1104067171
 61.5505819456 \times 65.0323767108 \times 69.3223609724
 73.8181868274 \times 77.3140530320 \times 81.7509854387
 86.2574385062 \times 89.7731713880 \times 94.2607686001
 98.7613544864 \times 102.2816371665 \times 106.7857859770
 111.2615741576 \times 114.7722598780 \times 119.2775293382
 123.6799886716 \times 127.1664954838 \times 131.6506912595
 and node2281 energy = 29.2094515 detHess 561.77
 0.2837920220 \times 4.7551866022 \times 8.2274941722
 12.6308620327 \times 17.0986768729 \times 20.5826601824
 25.0535028533 \times 29.4451899315 \times 32.9157923207
 37.3838804578 \times 41.5419321189 \times 45.0548268571
 49.4461339646 \times 53.1067395565 \times 57.0631871349
 61.5117512171 \times 64.9915749161 \times 69.3029367498
 73.8010938593 \times 77.2995963938 \times 81.7439554423
 86.2508204209 \times 89.7678872172 \times 94.2580490166
 98.7584800750 \times 102.2791803201 \times 106.7841830680


```

111.2592229983 × 114.7697795782 × 119.2751758965
123.6754217554 × 127.1615546587 × 131.6450354109
next globSP node3023 energy = 29.98039032 detHess - 39 886.79
- 2.9453930217 × 1.0448517399 × 5.8999466727
10.3811132346 × 14.0451953140 × 18.7050509931
23.2209040202 × 26.7943499125 × 31.3636752182
35.8807729612 × 39.4283530722 × 43.9634070542
48.4795720492 × 52.0187844435 × 56.5413895973
61.0567166301 × 64.5928470147 × 69.1109468747
73.6249552055 × 77.1593883739 × 81.6757584869
86.1864780823 × 89.7186086507 × 94.2340030748
98.7356213322 × 102.2623426932 × 106.7761988431
111.2521124625 × 114.7654443176 × 119.2740451035
123.6763705020 × 127.1642011140 × 131.6495616491
altGlobMin node3874 energy = 29.0613972 detHess - 383.26065
- 5.4360964470 - 0.5013984669 × 3.9526381429
7.6816435313 × 12.3958527509 × 16.9403683795
20.5415870250 × 25.1354723299 × 29.7320887350
33.3350850116 × 37.8780176768 × 42.5989035351
46.3372962726 × 50.7836420476 × 55.7252711928
59.9334386964 × 63.9008166123 × 68.7449007002
73.2272384299 × 76.8843440318 × 81.5378696891
86.0483476319 × 89.6178997012 × 94.1840510481
98.6865167083 × 102.2261908320 × 106.7581335945
111.2340887688 × 114.7525036428 × 119.2673635699
123.6693073826 × 127.1596324677 × 131.6471701046
(no SP in between !)
and node4442 energy = 29.05599100 detHess 1269.01
- 5.4518309320 - 0.5176868023 × 3.9215738270
7.6575578734 × 12.3743371295 × 16.9002598113
20.4969562682 × 25.0907271445 × 29.6424962327
33.2147231600 × 37.7610732816 × 42.3693452578
45.9785045790 × 50.4985341843 × 55.2495118815
59.0371569479 × 63.4324561430 × 68.3928961890
72.6923412309 × 76.5697318272 × 81.3684604880
85.8593231783 × 89.4896492837 × 94.1189294868
98.6197155780 × 102.1778981709 × 106.7331847102
111.2075940866 × 114.7324328209 × 119.2552212681
123.6530374806 × 127.1459900133 × 131.6351307205
and node4518 energy = 29.056364 detHess - 1241.220
- 5.4401604713 - 0.5104162098 × 3.9307713192
7.6621689096 × 12.3752570632 × 16.8983914512
20.4929899532 × 25.0849603295 × 29.6291678822
33.1966011777 × 37.7420954700 × 42.3305602382
45.9222951508 × 50.4466511861 × 55.1511874304
58.8706964443 × 63.3210650802 × 68.2413704065
72.3949689689 × 76.4106653598 × 81.2745027676
85.7425648150 × 89.4152813977 × 94.0807973883
98.5801051971 × 102.1507706798 × 106.7202354629

```

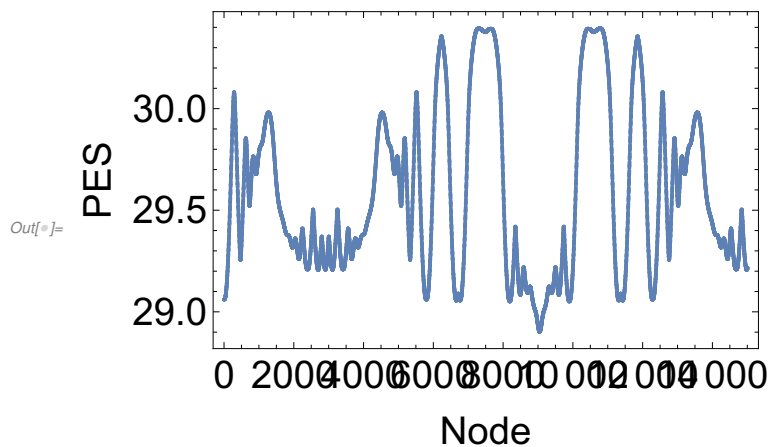
111.1959232555 \times 114.7257669564 \times 119.2539609702
 123.6559326253 \times 127.1518287663 \times 131.6443835873
 neuGlobSP ? node4864 energy = 30.39433316 detHess 259.76
 - 2.4158587651 \times 1.1004165302 \times 5.5081121549
 9.2160181843 \times 13.1311710179 \times 17.5815711233
 21.0774693076 \times 25.3651258621 \times 29.8830812554
 33.4017551370 \times 37.8355353064 \times 42.4053163894
 45.9751126974 \times 50.4571789344 \times 55.1297709653
 58.8138643325 \times 63.2664149580 \times 68.1399871318
 72.1857966852 \times 76.3023876512 \times 81.2049090020
 85.6487493258 \times 89.3575214432 \times 94.0505225498
 98.5475421928 \times 102.1284901946 \times 106.7090812595
 111.1847964715 \times 114.7183333789 \times 119.2506348326
 123.6534142784 \times 127.1511257888 \times 131.6455395829
 and node5105 energy = 30.39272865 detHess - 168.63359128
 - 2.3968926797 \times 1.1120011999 \times 5.5175120734
 9.2299706675 \times 13.1360070978 \times 17.5813695007
 21.0721695373 \times 25.3579626737 \times 29.8670786755
 33.3764323435 \times 37.8108104091 \times 42.3566551005
 45.9040013740 \times 50.3904108807 \times 55.0014243505
 58.6127133396 \times 63.1048028436 \times 67.8664661203
 71.6795948670 \times 76.0382661902 \times 80.9941671219
 85.3156603461 \times 89.1641814368 \times 93.9445932281
 98.4264422068 \times 102.0473724412 \times 106.6668279368
 111.1394934708 \times 114.6861207705 \times 119.2326145705
 123.6317396920 \times 127.1352342467 \times 131.6339704290
 mide gradMin node5466 3.7957581920301964 E - 002
 energy = 29.05175606 detHess - 56.23
 - 5.4202373498 - 0.4985007756 \times 3.9450846081
 7.6688424361 \times 12.3756555688 \times 16.8928988933
 20.4836261823 \times 25.0724288350 \times 29.6009545166
 33.1591267661 \times 37.7024918854 \times 42.2492370469
 45.8091123157 \times 50.3363991568 \times 54.9345435347
 58.5336221625 \times 63.0481606860 \times 67.7773249325
 71.5335260818 \times 75.9514439552 \times 80.8947925270
 85.1301723737 \times 89.0631889499 \times 93.8867747397
 98.3571457772 \times 102.0038913491 \times 106.6458536545
 111.1203126604 \times 114.6761471464 \times 119.2319692426
 123.6397849660 \times 127.1484468046 \times 131.6535176800
 neu Glob Min node6036 energy = 28.901986757 detHess 26762.87
 - 5.4539621038 - 0.5234364471 \times 3.9072078550
 7.6448647606 \times 12.3608265717 \times 16.8726826578
 20.4658369088 \times 25.0580170991 \times 29.5755415881
 33.1291722496 \times 37.6726899683 \times 42.1897887441
 45.7313586977 \times 50.2570888471 \times 54.7744254268
 58.3123776909 \times 62.8317914106 \times 67.3511434348
 70.8890633218 \times 75.4064268157 \times 79.9319934123
 83.4734501095 \times 87.9905584155 \times 92.5336282073
 96.0869315813 \times 100.6044847447 \times 105.1954920795

```

108.7876305740 × 113.2997913724 × 118.0130285858
121.7468490105 × 126.1806811805 × 131.1088339809
mild gradMin 3.7942171413964276 E - 002 node6603
energy = 29.05174665 detHess 62.33
-5.9896871900 - 1.4849421777 × 2.0234759786
6.4311883792 × 10.9863683451 × 14.5415851557
19.0161338922 × 23.6564947920 × 27.3013204574
31.7727316213 × 36.5934254437 × 40.5203450481
44.7621786852 × 49.7072083646 × 54.1225149174
57.8818720168 × 62.6131392851 × 67.1274310914
70.7273282735 × 75.3263825474 × 79.8536566026
83.4137458617 × 87.9608401188 × 92.5041801204
96.0623907453 × 100.5910658944 × 105.1798062749
108.7705519005 × 113.2878776515 × 117.9945954642
121.7183399866 × 126.1621793965 × 131.0841720706
next SP 6964 energy = 30.392729216 detHess - 162.37
-5.9665275746 - 1.4682897210 × 2.0350782217
6.4325958427 × 10.9789802007 × 14.5254635199
18.9975218635 × 23.6170141815 × 27.2379960456
31.7195485999 × 36.5000868373 × 40.3489173441
44.6699725333 × 49.6257852014 × 53.9846303569
57.7974636129 × 62.5589375406 × 67.0508647902
70.6620205146 × 75.2729305587 × 79.7588725413
83.3060141356 × 87.8517423149 × 92.2848560803
95.7938439942 × 100.3025790857 × 104.5849060461
108.0762727240 × 112.5204065374 × 116.4190877727
120.1385824112 × 124.5455944668 × 128.0533302395

```

NT33 predictor 0.01



```

neu Glob Min 6036 energy = 28.901986757 detHess 26 762.87
gMin = {-5.4539621038, -0.5234364471, 3.9072078550,
7.6448647606, 12.3608265717, 16.8726826578,
20.4658369088, 25.0580170991, 29.5755415881,
33.1291722496, 37.6726899683, 42.1897887441,
45.7313586977, 50.2570888471, 54.7744254268,
58.3123776909, 62.8317914106, 67.3511434348,
70.8890633218, 75.4064268157, 79.9319934123,
83.4734501095, 87.9905584155, 92.5336282073,
96.0869315813, 100.6044847447, 105.1954920795,
108.7876305740, 113.2997913724, 118.0130285858,
121.7468490105, 126.1806811805, 131.1088339809} + 2.0 * Pi

```

```

gMin = {0.8292232033795859, 5.759748860079586, 10.190393162179586,
13.928050067779587, 18.64401187887959, 23.155867964979585,
26.749022215979586, 31.341202406279585, 35.85872689527959,
39.41235755677959, 43.955875275479585, 48.472974051279586,
52.01454400487959, 56.54027415427959, 61.05761073397959, 64.59556299807959,
69.11497671777958, 73.63432874197957, 77.17224862897959, 81.6896121228796,
86.21517871947958, 89.75663541667959, 94.2737437226796, 98.81681351447958,
102.37011688847957, 106.88767005187958, 111.47867738667958,
115.07081588117958, 119.58297667957959, 124.29621389297958,
128.0300343176796, 132.46386648767958, 137.39201928807958`}

```

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

```
N = 33 new Glob minimum
```

```
k = 1.0
```

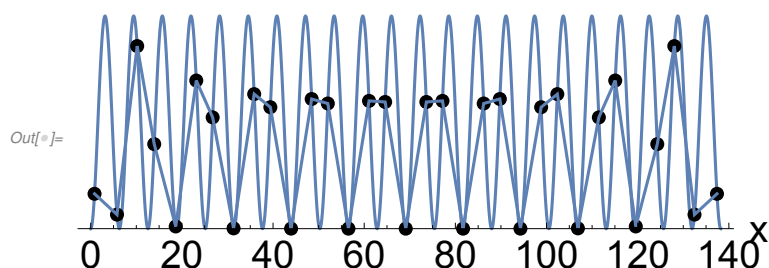
```
Setxx = gMin
```

```
Energy 28.901967932295
```

```
SetXX = {0.8337594996559949, 5.763013049869111, 10.195236981413217,
 13.930996211861586, 18.64557743389293, 23.157591724946624,
 26.750248950713576, 31.3418153976172, 35.85933852969872, 39.41281839994399,
 43.95610397112256, 48.47319935817806, 52.01472283218452, 56.54036736936191,
 61.057711606596065, 64.59565932460121, 69.11503837897544,
 73.63441743334967, 77.17236515135482, 81.68970938858898, 86.21535392576638,
 89.75687739977283, 94.27397278682834, 98.81725835800691,
 102.3707382282522, 106.8882613603337, 111.47982780723733,
 115.07248503300428, 119.58449932405797, 124.29908054608933,
 128.03483977653772, 132.4670637080818, 137.3963172582949`}
```

```
Eigenvalues
```

```
Out[*]= {4.31354, 4.29103, 4.25098, 4.19485, 4.12418, 4.04086, 3.9478, 3.85017, 3.75866,
 3.69454, 3.68446, 2.78803, 2.71392, 2.58859, 2.43713, 2.27238, 2.10149, 1.9298,
 1.76341, 1.61392, 1.51193, 1.21182, 1.21044, 0.744724, 0.63657, 0.525143,
 0.421415, 0.329295, 0.250681, 0.186806, 0.138916, 0.101916, 0.098355}
```



```
new glob SP 5105 energy = 30.39272865 detHess - 168.63359128
```

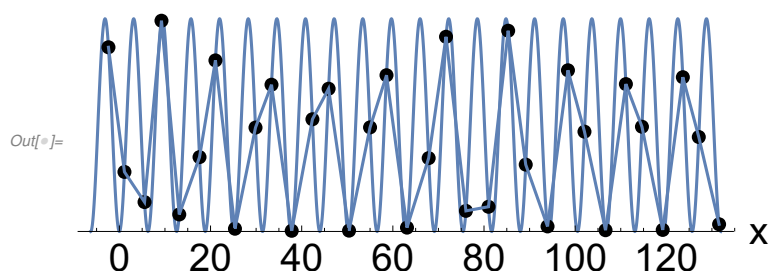
```
sp5105 = {-2.3968926797, 1.1120011999, 5.5175120734,
 9.2299706675, 13.1360070978, 17.5813695007,
 21.0721695373, 25.3579626737, 29.8670786755,
 33.3764323435, 37.8108104091, 42.3566551005,
 45.9040013740, 50.3904108807, 55.0014243505,
 58.6127133396, 63.1048028436, 67.8664661203,
 71.6795948670, 76.0382661902, 80.9941671219,
 85.3156603461, 89.1641814368, 93.9445932281,
 98.4264422068, 102.0473724412, 106.6668279368,
 111.1394934708, 114.6861207705, 119.2326145705,
 123.6317396920, 127.1352342467, 131.6339704290}
```

```
Setxx = sp5105
```

```
SetXX = {-2.3929651149721187, 1.1151911861770971, 5.52134241455561,
  9.237237573517408, 13.139575708486694, 17.584241487724128,
  21.07520513431296, 25.359306316286876, 29.86803922465918,
  33.377034533051926, 37.81082036292194, 42.35608252629719, 45.90287989053495,
  50.389123184541205, 54.99869242977604, 58.60847842403339,
  63.101060728799986, 67.85961074948796, 71.66747868438256, 76.0310030940211,
  80.98591582112095, 85.3000644038376, 89.15504111894623, 93.93855277310696,
  98.41774219330863, 102.04047295263571, 106.66132617259656,
  111.12994952127347, 114.65342338271142, 119.21054354941008,
  123.62492773215995, 127.12269946109654, 131.57748735045502`}
```

Eigenvalues

```
Out[*]= {4.32413, 4.28531, 4.24392, 4.18887, 4.11722, 4.0481, 3.95734, 3.86591, 3.81238,
  3.64835, 3.24084, 2.87724, 2.69231, 2.55656, 2.41515, 2.25981, 2.11519, 1.97586,
  1.81853, 1.70282, 1.56581, 1.40768, 0.693305, 0.582074, 0.487914, 0.357626,
  0.309898, 0.216271, -0.214437, 0.168342, 0.120985, 0.0795255, 0.00827453}
```



```
? new glob SP2 ? node4864 energy=30.39433316 detHess 259.76
```

```
NO is SP1 ? or 'very' flat in 2. direction ?
```

```
SP2at4864 = {-2.4158587651, 1.1004165302, 5.5081121549, 9.2160181843,
  13.1311710179, 17.5815711233, 21.0774693076, 25.3651258621, 29.883081255,
  33.4017551370, 37.8355353064, 42.4053163894, 45.9751126974, 50.4571789344,
  55.129770965, 58.8138643325, 63.266414958, 68.1399871318,
  72.1857966852, 76.3023876512, 81.2049090020, 85.6487493258, 89.3575214432,
  94.0505225498, 98.5475421928, 102.1284901946, 106.709081259,
  111.1847964715, 114.718333379, 119.250634833,
  123.6534142784, 127.15112578, 131.6455395829}
```

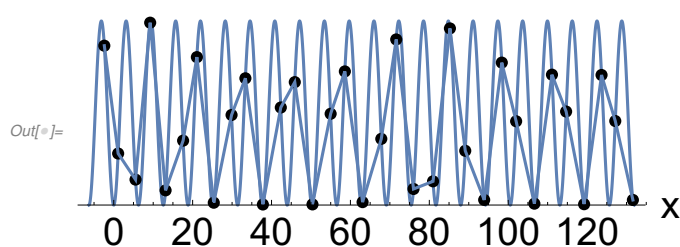
```
Setxx = SP2at4864
```

```
SetXX = {-2.3922534103279425, 1.1153816515524344, 5.521095430244578,
  9.236374451329487, 13.138944366885491, 17.58331138623005,
  21.073696954863195, 25.358137701981462, 29.86607127348669, 33.374224101068,
  37.80823310026338, 42.351146926244894, 45.895881495894734,
  50.38243729994399, 54.98568150225402, 58.58895620296225,
  63.084029092578625, 67.82861372761509, 71.61336024130563, 75.997922485057,
  80.94687858460095, 85.22559595967466, 89.11250678532095, 93.91132683932399,
  98.3800060614493, 102.01231171318972, 106.64061942262512,
  111.09626594265139, 114.68455683271922, 119.24697140516369,
  123.66649947331082, 127.14771077140834, 131.61322539108227`}
```

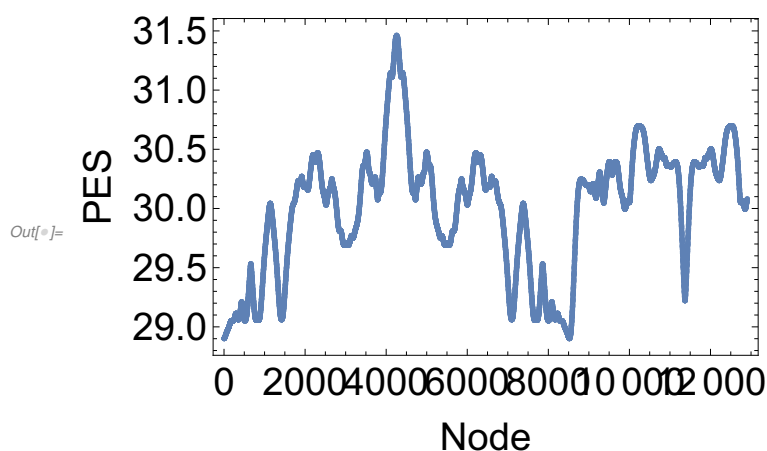
Eigenvalues

Out["]= {4.32337, 4.28451, 4.24235, 4.18763, 4.11722, 4.04863, 3.9564, 3.8695, 3.81085,
3.64786, 3.23282, 2.87532, 2.69162, 2.55563, 2.41296, 2.25762, 2.11457, 1.9738,
1.81793, 1.70907, 1.56475, 1.41189, 0.69645, 0.56304, 0.492021, 0.356758,
0.311232, 0.218262, -0.214124, 0.164439, 0.119548, 0.0796456, 0.00404466}

nextGlobSP3D



NT33 pr 0.015 from gMin direction Pull only



start energy before predictor 28.901986757635353 detHess 26 763.491

0.8292232034 × 5.7597488601 × 10.1903931622 × 13.9280500678

18.6440118789 × 23.1558679650 × 26.7490222160 × 31.3412024063

35.8587268953 × 39.4123575568 × 43.9558752755 × 48.4729740513

52.0145440049 × 56.5402741543 × 61.0576107340 × 64.5955629981

69.1149767178 × 73.6343287420 × 77.1722486290 × 81.6896121229

86.2151787195 × 89.7566354167 × 94.2737437227 × 98.8168135145
 102.3701168885 × 106.8876700519 × 111.4786773867 × 115.0708158812
 119.5829766796 × 124.2962138930 × 128.0300343177 × 132.4638664877
 137.3920192881
 SP Node 794 SP?nearby energy = 29.056396067 detHess - 1109.0
 0.8371335873 × 5.7686506316 × 10.2080378486
 13.9418318890 × 18.6566086219 × 23.1796330237
 26.7748527938 × 31.3675307099 × 35.9118316895
 39.4794739210 × 44.0252374984 × 48.6139282291
 52.2058781073 × 56.7303001472 × 61.4353575305
 65.1555668768 × 69.6054733145 × 74.5263893539
 78.6817949167 × 82.6956984207 × 87.5587073498
 92.0268824750 × 95.6990348121 × 100.3640506138
 104.8629260848 × 108.4332956889 × 113.0024967010
 117.4770009907 × 121.0063489817 × 125.5341831044
 129.9328560353 × 133.4281617024 × 137.9194625865
 Node 861 SP?nearby energy = 29.0559536 detHess 1357.87
 0.8380701177 × 5.7702139319 × 10.2115894067
 13.9448594650 × 18.6596953572 × 23.1858092827
 26.7818321323 × 31.3747915269 × 35.9266275123
 39.4987336706 × 44.0447733117 × 48.6532484786
 52.2625820621 × 56.7824162365 × 61.5338760854
 65.3223208739 × 69.7168471612 × 74.6775078498
 78.9782458657 × 82.8544658301 × 87.6526247186
 92.1438498646 × 95.7738562196 × 100.4028628147
 104.9041173847 × 108.4623629501 × 113.0176133623
 117.4932260279 × 121.0185076363 × 125.5415328140
 129.9426883683 × 133.4363036219 × 137.9266090127
 Node 2310 energy = 30.469369912 detHess - 467.2260
 0.8673679930 × 5.8187873014 × 10.3223219649
 14.0440587513 × 18.7614641006 × 23.3908915195
 27.0349129319 × 31.6245301120 × 36.4212412435
 40.2605492178 × 44.6480110072 × 49.6530935181
 54.0833521160 × 57.8877169403 × 62.6653483626
 67.2772433676 × 70.9245712730 × 75.5435366993
 80.3073042764 × 84.0903533650 × 88.5422431796
 93.5401887933 × 97.8881295605 × 101.7577357315
 106.5687464775 × 111.1368092307 × 114.7798602962
 119.4166762298 × 124.0896396802 × 127.7626084774
 132.2993402737 × 137.1812692044 × 141.1963688528
 Node 2962 energy = 29.6911575 detHess 215.477
 0.9064822844 × 5.8826123656 × 10.4687964543
 14.1905490415 × 18.9108771428 × 23.6924880415
 27.4826076022 × 31.9842944105 × 37.0242384613
 41.4393840522 × 45.2909774715 × 50.1084147219
 54.7694292579 × 58.4520893231 × 63.0799377847
 67.9533340076 × 71.9092478308 × 76.2056001414
 81.2244282057 × 85.8020155553 × 89.5496552133
 94.2971931339 × 99.0941244742 × 102.9000144959

107.4038632022 × 112.4638344119 × 116.9318354812
 120.7610598193 × 125.5722397582 × 130.2920807947
 134.0154489595 × 138.6174708325 × 143.5972695884
 Node 3030 energy = 29.6915609 detHess - 127.34044
 0.9102945385 × 5.8887692204 × 10.4829747290
 14.2057077228 × 18.9260927166 × 23.7229398034
 27.5327186013 × 32.0179772649 × 37.0695697531
 41.5323875491 × 45.3573710175 × 50.1632619110
 54.8671101828 × 58.5770862139 × 63.1841678625
 68.1363208492 × 72.2586915129 × 76.3790016978
 81.3302423718 × 85.9374895794 × 89.6470515175
 94.3503858531 × 99.1561464883 × 102.9810494074
 107.4436519475 × 112.4949965530 × 116.9797697910
 120.7896338550 × 125.5864556223 × 130.3061036792
 134.0282001375 × 138.6227908665 × 143.6000789108
 Node 3073 energy = 29.69155357 detHess 162.9
 0.9138297454 × 5.8944683843 × 10.4961056502
 14.2199057294 × 18.9402849072 × 23.7512686456
 27.5801206564 × 32.0487536239 × 37.1088133567
 41.6122640668 × 45.4184607534 × 50.2156081361
 54.9629018716 × 58.7103076489 × 63.2881844872
 68.3067192081 × 72.6021267062 × 76.5588711023
 81.4326769540 × 86.0603075877 × 89.7430326736
 94.4042774936 × 99.2213821678 × 103.0724095631
 107.4882015797 × 112.5281500204 × 117.0291523121
 120.8196435969 × 125.6014784356 × 130.3211257191
 134.0422834399 × 138.6289676910 × 143.6040485266
 Node 5450 energy = 29.69167579 detHess 193.5
 0.9138461345 × 5.8944947824 × 10.4961664862
 14.2199718669 × 18.9403508782 × 23.7514001494
 27.5803424499 × 32.0488952303 × 37.1089889557
 41.6126195504 × 45.4187413462 × 50.2158514622
 54.9633509560 × 58.7109558702 × 63.2886705716
 68.3074794493 × 72.6036864231 × 76.5597631578
 81.4332566865 × 86.0611369302 × 89.7438404714
 94.4048968975 × 99.2224249820 × 103.0741456230
 107.4891973480 × 112.5291831805 × 117.0310934240
 120.8211280665 × 125.6027000717 × 130.3233038393
 134.0453007432 × 138.6313089839 × 143.6078702261
 Node 5495 energy = 29.692092707 detHess - 111.36
 0.9102770202 × 5.8887409544 × 10.4829096195
 14.2056377043 × 18.9260225820 × 23.7227996232
 27.5324859143 × 32.0178236312 × 37.0693685448
 41.5319761419 × 45.3570663204 × 50.1630046223
 54.8666443604 × 58.5764634553 × 63.1836631385
 68.1354603937 × 72.2569954240 × 76.3781660629
 81.3298019735 × 85.9370309295 × 89.6467768086
 94.3503256582 × 99.1562409290 × 102.9813168780
 107.4438863966 × 112.4953874745 × 116.9806393525

120.7903406617 \times 125.5871132091 \times 130.3073676884
 134.0299829685 \times 138.6242199984 \times 143.6024742900
 Node 5561 energy = 29.6915084 detHess 270.97
 0.9064950036 \times 5.8826329263 \times 10.4688437898
 14.1905993548 \times 18.9109277480 \times 23.6925894487
 27.4827730169 \times 31.9844075997 \times 37.0243948152
 41.4397056573 \times 45.2911986852 \times 50.1085928426
 54.7697402161 \times 58.4524688176 \times 63.0802618330
 67.9539167240 \times 71.9103211617 \times 76.2061546738
 81.2248472306 \times 85.8026751394 \times 89.5501875939
 94.2975905753 \times 99.0947839290 \times 102.9010242534
 107.4044997810 \times 112.4646267601 \times 116.9334223854
 120.7622211326 \times 125.5731944364 \times 130.2937795666
 134.0177507097 \times 138.6192742418 \times 143.6002438122
 Node 6213 energy = 30.4701332 detHess - 494.724
 0.8673746368 \times 5.8187982425 \times 10.3223469858
 14.0440822509 \times 18.7614882635 \times 23.3909404148
 27.0349782379 \times 31.6245905798 \times 36.4213560295
 40.2607514732 \times 44.6481315590 \times 49.6532271729
 54.0836082457 \times 57.8878958078 \times 62.6654910341
 67.2774905434 \times 70.9248577682 \times 75.5437947250
 80.3077891342 \times 84.0911599236 \times 88.5427716214
 93.5408817435 \times 97.8895137688 \times 101.7585960757
 106.5693727856 \times 111.1378090938 \times 114.7808542901
 119.4175530371 \times 124.0912755211 \times 127.7649993406
 132.3012789396 \times 137.1845745199 \times 141.2026935970
 Node 7097 energy = 29.062366031 detHess 244.05
 0.8440434880 \times 5.7801695960 \times 10.2342258139
 13.9643756722 \times 18.6796342252 \times 23.2257876045
 26.8279117903 \times 31.4223114661 \times 36.0230960288
 39.6294110565 \times 44.1717979125 \times 48.9025533863
 52.6548355785 \times 57.0903934609 \times 62.0415667135
 66.2821851708 \times 70.2189457021 \times 75.0486791325
 79.5359426249 \times 83.1838344177 \times 87.8293898307
 92.3401523262 \times 95.9071080561 \times 100.4701473768
 104.9724066442 \times 108.5111481093 \times 113.0419367211
 117.5173548572 \times 121.0352094150 \times 125.5495470811
 129.9499734823 \times 133.4398241997 \times 137.9266450799
 bad : an der Spitze gespiegelt ! Node 7103
 Node 7663 energy = 29.057083
 Node 7730 energy = 29.0575132 detHess - 1408.328
 0.8371316854 \times 5.7686474563 \times 10.2080306357
 13.9418257497 \times 18.6566023646 \times 23.1796205071
 26.7748386875 \times 31.3675160190 \times 35.9118017403
 39.4794351468 \times 44.0251979650 \times 48.6138484396
 52.2057645013 \times 56.7301937580 \times 61.4351537181
 65.1552303165 \times 69.6052340951 \times 74.5260364396
 78.6811012819 \times 82.6953507548 \times 87.5585219562
 92.0266890297 \times 95.6989504159 \times 100.3640651984

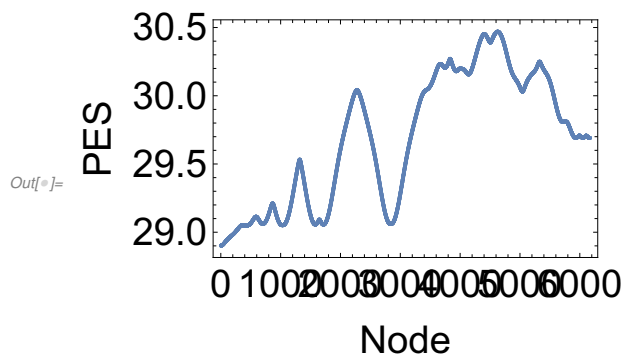
104.8630540322 × 108.4334894976 × 113.0027469853
 117.4775569132 × 121.0070291140 × 125.5349498054
 129.9344696219 × 133.4299313356 × 137.9215449233
 Node 8521 glob Min energy = 28.90328599 detHess 27 008.08
 0.8337594971 × 5.7630130456 × 10.1952369718
 13.9309962038 × 18.6455774257 × 23.1575917086
 26.7502489326 × 31.3418153786 × 35.8593384909
 39.4128183516 × 43.9561039201 × 48.4731992536
 52.0147226970 × 56.5403672275 × 61.0577113163
 64.5956589445 × 69.1150379820 × 73.6344166225
 77.1723640821 × 81.6897082769 × 86.2153516600
 89.7568743821 × 94.2739696802 × 98.8172520567
 102.3707296299 × 106.8882527498 × 111.4798105976
 115.0724600279 × 119.5844763609 × 124.2990371378
 128.0347670377 × 132.4670138336 × 137.3962469699
 Node 8814 energy = 30.248412 detHess - 4796.9199
 0.8336779174 × 5.7628766339 × 10.1949273638
 13.9307356047 × 18.6453124543 × 23.1570628939
 26.7496644517 × 31.3412023528 × 35.8580855910
 39.4112592866 × 43.9544595356 × 48.4698257652
 52.0103667439 × 56.5357926455 × 61.0483437838
 64.5834331495 × 69.1022255912 × 73.6082055958
 77.1381186124 × 81.6537684964 × 86.1417814031
 89.6613827653 × 94.1730576119 × 98.6100799767
 102.1077600170 × 106.6054220648 × 110.8958682824
 114.3786824426 × 118.8198977745 × 122.7293991192
 126.4330960673 × 130.8324901442 × 134.3342371257
 Node 9509 energy = 30.3952880540 detHess 545.16070350
 0.8285552081 × 5.7543009591 × 10.1754762756
 13.9145020492 × 18.6288402492 × 23.1242504592
 26.7139293837 × 31.3035543136 × 35.7810433689
 39.3182278329 × 43.8542451290 × 48.2625600689
 51.7627976058 × 56.2603366154 × 60.4735229634
 63.9811142517 × 68.4011674325 × 72.1664561549
 76.0217975950 × 80.4610792062 × 83.9611481822
 88.2202676885 × 92.7322841591 × 96.2458293336
 100.6694818055 × 105.2312086405 × 108.7930092281
 113.2727011512 × 117.9268612378 × 121.5878739902
 126.0530339890 × 130.8977606352 × 134.8754968645
 Node 9651 energy = 30.3941876547 detHess - 87.11
 0.8245730600 × 5.7476212770 × 10.1603433181
 13.9020589114 × 18.6162636863 × 23.0992866401
 26.6874403913 × 31.2754645859 × 35.7234882504
 39.2523414710 × 43.7810404011 × 48.1098384597
 51.6048403261 × 56.0731796442 × 60.0837464876
 63.7109029353 × 68.1081925336 × 71.6603320679
 75.7740556192 × 80.2548256928 × 83.7459764551
 88.1176790126 × 92.6418690607 × 96.1666755497
 100.6315046927 × 105.1967043189 × 108.7629918393

```

113.2586672624 × 117.9149754738 × 121.5768174566
126.0493297372 × 130.8979790270 × 134.8797467504
Node 9676 node = 10 737 energy = 30.502849557340
detHess - 44.63367
0.3650975835 × 4.9109282362 × 8.4764031517
12.8543471521 × 17.5163038232 × 21.2063417057
25.6030681378 × 30.4529722928 × 34.4819941394
38.5864692569 × 43.4663501352 × 47.8528722051
51.5732832737 × 56.2593098983 × 60.6599996775
64.2359511679 × 68.7980406531 × 73.0484148560
76.5871813815 × 81.0539289873 × 84.9335699281
88.7028677393 × 93.1451774465 × 96.6951024820
100.8848519377 × 105.4211479643 × 108.9732077653
113.3571743803 × 117.9980658109 × 121.6566410976
126.0766179756 × 130.8978729896 × 134.8521935812

```

NT33 pr 0.0075 gMin direction Pull



```

start detHess 26 763.49 energy = 28.9019834
0.8292232034 × 5.7597488601 × 10.1903931622 × 13.9280500678
18.6440118789 × 23.1558679650 × 26.7490222160 × 31.3412024063
35.8587268953 × 39.4123575568 × 43.9558752755 × 48.4729740513
52.0145440049 × 56.5402741543 × 61.0576107340 × 64.5955629981
69.1149767178 × 73.6343287420 × 77.1722486290 × 81.6896121229
86.2151787195 × 89.7566354167 × 94.2737437227 × 98.8168135145
102.3701168885 × 106.8876700519 × 111.4786773867 × 115.0708158812
119.5829766796 × 124.2962138930 × 128.0300343177 × 132.4638664877
137.3920192881
mild grad - min 2.8684218066 E - 002
node1032 energy = 29.0514251 detHess 1.248
?BBP point crossed?
0.8351666901 5.7653699802 × 10.2005889033
13.9355073246 × 18.6501631989 × 23.1667449149
26.7604067644 × 31.3524520350 × 35.8810654159
39.4400896559 × 43.9846680426 × 48.5316173200
52.0918326896 × 56.6195716726 × 61.2181551864
64.8176586906 × 69.3322748286 × 74.0624228414
77.8200554583 × 82.2368930897 × 87.1810853941
91.4195080843 × 95.3497108593 × 100.1719953496
104.6429701373 × 108.2888260015 × 112.9300659998

```

117.4048153242 × 120.9604261007 × 125.5159958714
 129.9243918052 × 133.4330818621 × 137.9381957172
 node1581 energy = 29.05634549 detHess - 1200.28
 0.8371357898 × 5.7686589937 × 10.2080583635
 13.9418447905 × 18.6566182882 × 23.1796489102
 26.7748687445 × 31.3675456078 × 35.9118604109
 39.4795101829 × 44.0252739752 × 48.6140013819
 52.2059814589 × 56.7303970851 × 61.4355435565
 65.1558727636 × 69.6056916770 × 74.5267137737
 78.6824311512 × 82.6960152472 × 87.5588752485
 92.0270546874 × 95.6991043179 × 100.3640275169
 104.8627874086 × 108.4330917843 × 113.0022382894
 117.4764307572 × 121.0056527314 × 125.5333992650
 129.9312072920 × 133.4263556525 × 137.9173362129
 and node1718 energy = 29.0559659 detHess 1319.1
 0.8380731005 × 5.7702236369 × 10.2116129796
 13.9448748625 × 18.6597074879 × 23.1858300232
 26.7818535677 × 31.3748120272 × 35.9266675584
 39.4987852090 × 44.0448247181 × 48.6533510706
 52.2627314832 × 56.7825507542 × 61.5341265889
 65.3227548641 × 69.7171194189 × 74.6778428091
 78.9788951385 × 82.8548416408 × 87.6528726097
 92.1442056650 × 95.7741388614 × 100.4030851546
 104.9044998918 × 108.4627780996 × 113.0180292269
 117.4940571335 × 121.0194955083 × 125.5426106640
 129.9449260660 × 133.4387636785 × 137.9294902150
 and node2834 energy = 29.06140997 detHess - 291.8448
 0.8436076731 × 5.7794488110 × 10.2325874438
 13.9629457803 × 18.6781677571 × 23.2228393710
 26.8244582253 × 31.4187750837 × 36.0159404865
 39.6194130773 × 44.1624284674 × 48.8846027533
 52.6247557329 × 57.0698367388 × 62.0128130389
 66.2252955967 × 70.1885794553 × 75.0307620553
 79.5136959607 × 83.1695542222 × 87.8220006657
 92.3323360167 × 95.9014754196 × 100.4671813893
 104.9691470365 × 108.5084720834 × 113.0401776283
 117.5147563806 × 121.0325236977 × 125.5469967409
 129.9450251140 × 133.4345292778 × 137.9205778961
 and node2852 energy = 29.0613888218 detHess 346.017
 0.8440576610 × 5.7801979865 × 10.2342919755
 13.9644282478 × 18.6796843468 × 23.2258846329
 26.8280233219 × 31.4224237626 × 36.0233213843
 39.6297258272 × 44.1720913161 × 48.9031135702
 52.6557782767 × 57.0910303912 × 62.0424435091
 66.2839190537 × 70.2198850011 × 75.0492462881
 79.5366705078 × 83.1843275544 × 87.8296818702
 92.3405326010 × 95.9074506917 × 100.4704221758
 104.9728878860 × 108.5117070640 × 113.0425028880
 117.5184935431 × 121.0365928792 × 125.5510615479

```

129.9531236882 × 133.4433118589 × 137.9307370516
glob SP node4628 energy = 30.46925611579 detHess - 484.0
0.8673733724 × 5.8188011311 × 10.3223553374
14.0440843756 × 18.7614866852 × 23.3909335342
27.0349665942 × 31.6245782415 × 36.4213309271
40.2607062196 × 44.6481043546 × 49.6531966327
54.0835493728 × 57.8878539999 × 62.6654567838
67.2774300639 × 70.9247870036 × 75.5437304408
80.3076677682 × 84.0909575253 × 88.5426387812
93.5407074035 × 97.8891650934 × 101.7583790269
106.5692145622 × 111.1375560352 × 114.7806017536
119.4173295573 × 124.0908577726 × 127.7643868677
132.3007815144 × 137.1837264256 × 141.2010687841
iMin node5935 energy = 29.6908884 detHess 232.68
0.9065061925 × 5.8826562236 × 10.4688995003
14.1906519476 × 18.9109770485 × 23.6926846900
27.4829256505 × 31.9845109907 × 37.0245361235
41.4399951368 × 45.2913965695 × 50.1087505265
54.7700134479 × 58.4528007339 × 63.0805440119
67.9544226796 × 71.9112525136 × 76.2066352790
81.2252092084 × 85.8032432289 × 89.5506450541
94.2979309145 × 99.0953470922 × 102.9018857081
107.4050417996 × 112.4652997733 × 116.9347690506
120.7632071833 × 125.5740048006 × 130.2952212032
134.0197056253 × 138.6208038701 × 143.6027632807
and node6053 energy = 29.69132903 detHess - 138.8298
and node6166 energy = 29.6908971 detHess 237.36
ok alterniert am Grund

```

```

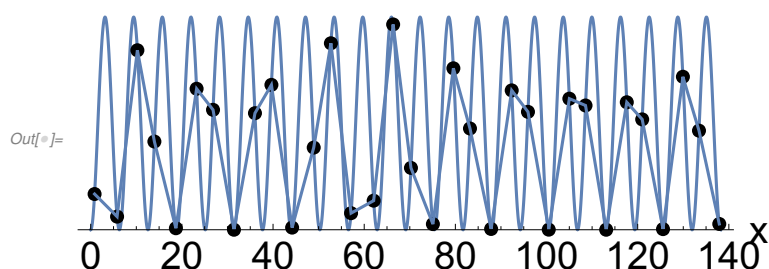
SD at glob SP goes to 29.06354744 also not to glob min
IRCfin = {0.84717010141546789, 5.7868292717828265, 10.246156518285151,
13.977529161088009, 18.687062326163048, 23.249759452084234,
26.849220697084910, 31.452350736703306, 36.066644875506306,
39.700650826448374, 44.223248509122406, 49.017665668766838,
52.835334617440466, 57.212187124573184, 62.165469331047873,
66.537214789141913, 70.351969622102018, 75.136474766538385,
79.628845160560545, 83.252316345158235, 87.857104138549985,
92.378153517103954, 95.929444105598563, 100.48662783660929,
104.98315706619766, 108.52252660629053, 113.04453891034451,
117.52370481872019, 121.03800516475189, 125.55277253740810,
129.95197887617206, 133.44196879119815, 137.92787811943344}
Setxx = IRCfin

```

```
SetXX = {0.8445625285392737, 5.781033410443023, 10.236191398176846,
 13.96608837247976, 18.68138706567522, 23.22930844020367, 26.832045085189264,
 31.42653599459283, 36.031636163657886, 39.64140614228187, 44.18296073074015,
 48.92383495925797, 52.69084909755673, 57.114405914073195, 62.07400183329639,
 66.34623539635975, 70.2542540513897, 75.0705783921981, 79.56508825252698,
 83.2047428053583, 87.84327122446174, 92.36077398010866, 95.92785571327991,
 100.48897235126981, 105.0081087660103, 108.55478794526185,
 113.08707871195386, 117.60911284120637, 120.98949416030854,
 125.55544014510328, 129.921325116795, 133.4498893627599, 137.89871353160228`}
```

Eigenvalues

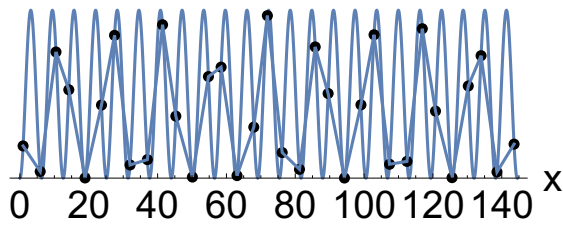
```
Out[*]= {4.32843, 4.29685, 4.261, 4.20602, 4.13238, 4.05922, 3.95567, 3.89305, 3.79045,
 3.71175, 3.21708, 2.90022, 2.73757, 2.61855, 2.46304, 2.29681, 2.13456,
 1.94271, 1.81462, 1.60331, 1.52652, 1.42879, 1.19499, 0.706255, 0.545803,
 0.507055, 0.35407, 0.306393, 0.2214, 0.172686, 0.137964, 0.107584, 0.00723928}
```



```
Node 2962 energy = 29.6911575 detHess 215.477 new iMin
iMin2962 = {0.9064822844, 5.8826123656, 10.4687964543,
 14.1905490415, 18.9108771428, 23.6924880415,
 27.4826076022, 31.9842944105, 37.0242384613,
 41.4393840522, 45.2909774715, 50.1084147219,
 54.7694292579, 58.4520893231, 63.0799377847,
 67.9533340076, 71.9092478308, 76.2056001414,
 81.2244282057, 85.8020155553, 89.5496552133,
 94.2971931339, 99.0941244742, 102.9000144959,
 107.4038632022, 112.4638344119, 116.9318354812,
 120.7610598193, 125.5722397582, 130.2920807947,
 134.0154489595, 138.6174708325, 143.5972695884}
Setxx = iMin2962
```

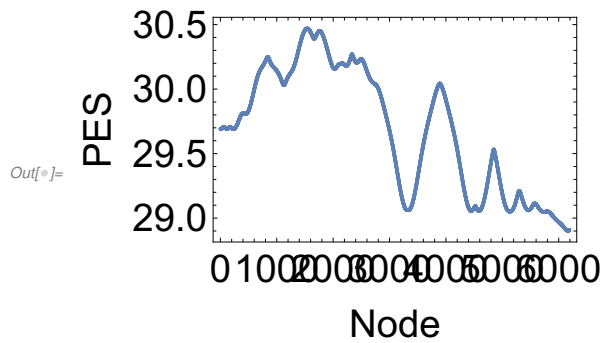
Eigenvalues

```
{4.351003612538189, 4.328984476457263, 4.289924428375925, 4.225680835943325,
4.163378046559696, 4.1074964663349105, 4.023345786328811, 3.9466549230908194,
3.804494200139155, 3.7930097704674814, 3.0120750306605224,
2.9272939884059777, 2.8037555600593693, 2.6232316501241035,
2.470973309455883, 2.3276900631408703, 2.15253824732865, 1.9812239261896254,
1.7381693176028672, 1.6869902539447974, 1.5181116473138219,
1.4244823894442615, 1.1143098927225288, 1.0933388364845404,
0.435613828067408, 0.38038758757708235, 0.32125135944805994,
0.28401050380786597, 0.18291364533358134, 0.1617995658403606,
0.064214746300431, 0.04681338514882061, 0.01135843685688975}
```

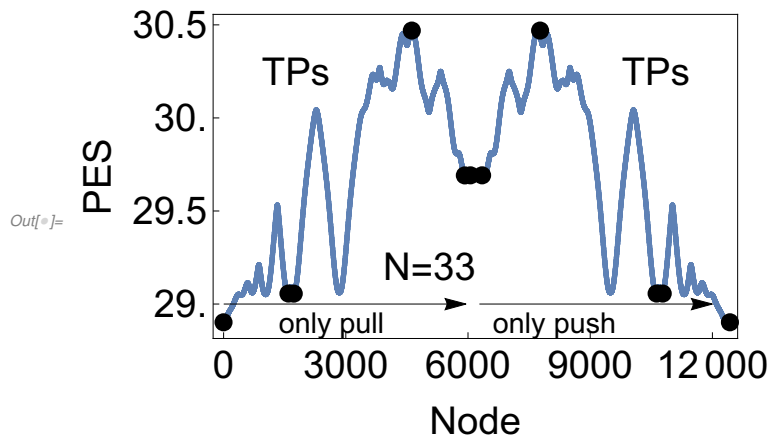


it is not fully symmetric

NT33 pr 0.0075 from iMin direction Push



Join[NT33pr0p0075gMinPull, NT33pr0p0075iMinPush]




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

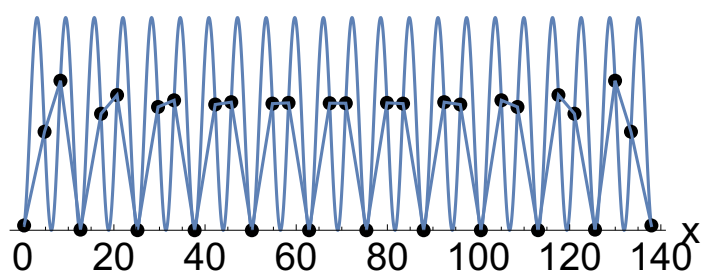
N = 34 a_o minimum

ENERGY 29.726839613975546

```
SetXX = {0.30057574360883743, 4.785436007386995, 8.27296297300696,
  12.673993680456853, 17.182439871834465, 20.69552152726902,
  25.170982506970738, 29.684675238424724, 33.2112134192558, 37.71265961338234,
  42.227653162464414, 45.759498928714244, 50.27011875561789,
  54.78537509687975, 58.3191018042001, 62.83296680280151, 67.34794571987119,
  70.88212912649313, 75.39710863794747, 79.91097325014567, 83.4446998589594,
  87.95995681235468, 92.47057632629298, 96.00242216007967, 100.51741601217162,
  105.01886173730617, 108.5454000079017, 113.05909339235194,
  117.53455395272718, 121.04763567093333, 125.55608248680015,
  129.95711332708262, 133.44464046988446, 137.92950094018957`}
```

Eigenvalues

```
{4.31127, 4.28673, 4.24734, 4.19371, 4.12684, 4.04837, 3.96098, 3.86931, 3.78216,
  3.71641, 3.21755, 3.21722, 2.75971, 2.65184, 2.51212, 2.35629, 2.1927, 2.02679,
  1.86324, 1.7077, 1.5701, 1.44369, 1.43346, 0.782245, 0.71291, 0.617745,
  0.518366, 0.424398, 0.340168, 0.267947, 0.209074, 0.164357, 0.134031, 0.11725}
```



start energy 29.72684059070

```
0.3067969756 × 4.7916609756 × 8.2791809756
12.6802209756 × 17.1886209756 × 20.7017209756
25.1772209756 × 29.6909209756 × 33.2174209756
37.7189209756 × 42.2339209756 × 45.7657209756
50.2763209756 × 54.7916209756 × 58.3253209756
62.8392209756 × 67.3541209756 × 70.8883209756
75.4033209756 × 79.9172209756 × 83.4509209756
87.9662209756 × 92.4768209756 × 96.0086209756
100.5232209756 × 105.0252209756 × 108.5512209756
113.0652209756 × 117.5412209756 × 121.0542209756
125.5622209756 × 129.9632209756 × 133.4512209756
137.9362209756
```

SP node276 energy = 30.15284614 detHess - 87.86

```
0.8257593800 × 5.7535759742 × 10.1761963361
13.9161408145 × 18.6317582973 × 23.1312959773
26.7221386168 × 31.3128082615 × 35.8005422840
39.3415147404 × 43.8799245417 × 48.3161404542
51.8231532749 × 56.3300799575 × 60.6201553895
64.1086736747 × 68.5542913983 × 72.4680901890
76.1720022021 × 80.5747571150 × 84.0833071407
88.2659194490 × 92.7453176667 × 96.2270497702
```

100.6265099716 × 105.1213699264 × 108.6236607044
 113.0975943028 × 117.5717866747 × 121.0741529553
 125.5689844014 × 129.9692356857 × 133.4511188149
 137.9307870487
 SP node476 energy = 30.9278526084 detHess - 36 381.14233
 0.8456934426 × 5.7714220850 × 10.2074353976
 13.9382825687 × 18.6494173487 × 23.1617469892
 26.7530927245 × 31.3432108537 × 35.8606773654
 39.4137456900 × 43.9564872214 × 48.4734216894
 52.0147354267 × 56.5401679915 × 61.0571008856
 64.5947607762 × 69.1140239609 × 73.6322727277
 77.1695037992 × 81.6867052203 × 86.2092028435
 89.7486898223 × 94.2655146445 × 98.8000735737
 102.3474203615 × 106.8647443899 × 111.4326410040
 115.0049428158 × 119.5210580012 × 124.1772481902
 127.8369927523 × 132.3206642526 × 137.1694660893
 141.1456140674
 node813 energy = 30.01839758 detHess 1758.744
 0.8295170530 × 5.7619756245 × 10.1965046361
 13.9336598488 × 18.6501788618 × 23.1686391055
 26.7634521664 × 31.3564708838 × 35.8900689720
 39.4519137777 × 43.9972412347 × 48.5575122198
 52.1271768022 × 56.6548280836 × 61.2884403916
 64.9224276082 × 69.4243441864 × 74.2306582246
 78.1171742321 × 82.4138617459 × 87.3792446153
 91.7921365994 × 95.5716204339 × 100.3207654199
 104.8612553978 × 108.4738611600 × 113.0825166217
 117.6763537183 × 121.2790715232 × 125.8285569696
 130.5421475971 × 134.2694932868 × 138.7272959483
 143.6620819079

 start energy before predictor 29.72684059
 0.3005746368 × 4.7854387742 × 8.2729538811
 12.6739911649 × 17.1824431594 × 20.6955142871
 25.1709819227 × 29.6846816100 × 33.2112096558
 37.7126617320 × 42.2276635642 × 45.7594999627
 50.2701257316 × 54.7853948914 × 58.3191147800
 62.8329861928 × 67.3479908055 × 70.8821757420
 75.3971629019 × 79.9110893196 × 83.4448393518
 87.9601077017 × 92.4708894557 × 96.0028193484
 100.5178378753 × 105.0197296245 × 108.5465093922
 113.0602747482 × 117.5369874782 × 121.0506564724
 125.5593998629 × 129.9640257460 × 133.4523567893
 137.9385559580
 SP node518 energy = 30.5185048 detHess 145.289098
 0.3039600217 × 4.7920512593 × 8.2833138585
 12.6838203809 × 17.2015068301 × 20.7221757905
 25.1976407583 × 29.7379597063 × 33.2840159183
 37.7862050750 × 42.3753774017 × 45.9652021083

50.4713050793 × 55.1817805383 × 58.9129735240
 63.3455145592 × 68.2694251049 × 72.4449576299
 76.4332748121 × 81.2814804508 × 85.7403335647
 89.4052042665 × 94.0616126861 × 98.5329276881
 102.0941302135 × 106.6553036227 × 111.0582975996
 114.5689283131 × 119.0746423893 × 123.2792255021
 126.7969833575 × 131.2205467985 × 134.9799689253
 138.8476933856

node881 energy = 30.39412799 detHess - 6.45058

0.3109719523 × 4.8057462720 × 8.3048752196
 12.7040622311 × 17.2405061895 × 20.7776817202
 25.2516914944 × 29.8443712249 × 33.4370512434
 37.9300354814 × 42.6518964612 × 46.4025135864
 50.8135494069 × 55.7456235078 × 59.9582238910
 63.9060561349 × 68.7330991214 × 73.1874214173
 76.8396515038 × 81.4835251491 × 85.9308038805
 89.4833633507 × 94.0345697075 × 98.3741778621
 101.8806214181 × 106.3627130464 × 110.4085454895
 114.0168905045 × 118.4205674559 × 122.0050795770
 126.0838956269 × 130.5706451376 × 134.0762598858
 138.4298873574

node1056 energy = 30.662526966 detHess - 364.8562

0.3304186533 × 4.8329219008 × 8.3413736750
 12.7386381100 × 17.2960927321 × 20.8536467633
 25.3234639947 × 29.9716687757 × 33.6265720132
 38.0902313186 × 42.9244844092 × 46.8825392614
 51.0895838240 × 56.0224114985 × 60.4444657791
 64.1909701979 × 68.9108148803 × 73.4187389419
 77.0157236470 × 81.6095265727 × 86.1222702453
 89.6770664339 × 94.2205158672 × 98.7280864945
 102.2657327175 × 106.7913587116 × 111.2845859577
 114.8013905423 × 119.3201941234 × 123.7665556179
 127.2361369659 × 131.7537527677 × 136.0695862684
 139.4946257120

new Pred 0.04 PULL only start at gMin stepmax = 1.0 eps 1 * 10⁻¹¹

SP node392 energy = 31.081595809 detHess - 1457.61557

0.3025287952 × 4.7892541096 × 8.2789320938
 12.6796692363 × 17.1934627618 × 20.7108918571
 25.1864103861 × 29.7155723116 × 33.2531151288
 37.7553848641 × 42.3138979258 × 45.8771703701
 50.3883878933 × 55.0222016561 × 58.6569978422
 63.1507680874 × 67.9580748026 × 71.8497951975
 76.1372210083 × 81.0981939458 × 85.5084565163
 89.2856938812 × 94.0319186496 × 98.5639549330
 102.1734623561 × 106.7804003554 × 111.3535948949
 114.9417070636 × 119.4926303509 × 124.1554284581
 127.8201802190 × 132.3182696220 × 137.1792590200
 141.1724185996

end fine moved

node422 ? mirror energy = 31.081662 detHess 1579.61837

0.3030883064 × 4.7903476757 × 8.2806442853

12.6812928233 × 17.1966107721 × 20.7153010383

25.1908083343 × 29.7243501098 × 33.2651769389

37.7674852825 × 42.3381138046 × 45.9114339456

50.4212342314 × 55.0861573342 × 58.7569376280

63.2313199106 × 68.0946294061 × 72.1056169085

76.2670452029 × 81.1920419864 × 85.6469714867

89.3680526167 × 94.0751653827 × 98.6105198404

102.2063811996 × 106.7967748808 × 111.3697940950

114.9550726926 × 119.4994654550 × 124.1625225666

127.8280016673 × 132.3224695472 × 137.1837478180

141.1794353173

node638 energy = 31.07784988 detHess - 1658.7796

0.3057825945 × 4.7956123579 × 8.2889031881

12.6890971158 × 17.2117096967 × 20.7365692799

25.2118474816 × 29.7661494569 × 33.3235687907

37.8247899413 × 42.4513586040 × 46.0787214830

50.5710933682 × 55.3643410878 × 59.2313433160

63.5413230577 × 68.5027345365 × 72.8893917373

76.6846757027 × 81.4398054664 × 85.9556753435

89.5659955063 × 94.1758473764 × 98.7138290316

102.2819991501 × 106.8339703408 × 111.4057603527

114.9848352677 × 119.5141774374 × 124.1767786212

127.8428947322 × 132.3295788222 × 137.1896777059

141.1871704229

node726 mirror ? energy = 31.078174 detHess 1839.35751

0.3079132603 × 4.7997741665 × 8.2954507290

12.6952522331 × 17.2235788548 × 20.7534275473

25.2283175820 × 29.7986385242 × 33.3700400100

37.8688706266 × 42.5366458480 × 46.2122414935

50.6783514492 × 55.5457003009 × 59.5699785476

63.7142488404 × 68.6307822654 × 73.0817655576

76.7981097913 × 81.4998843902 × 86.0211296531

89.6110157942 × 94.1980437150 × 98.7353562456

102.2978328186 × 106.8411488623 × 111.4114602663

114.9883859467 × 119.5144670861 × 124.1740942995

127.8370151633 × 132.3238502650 × 137.1787798835

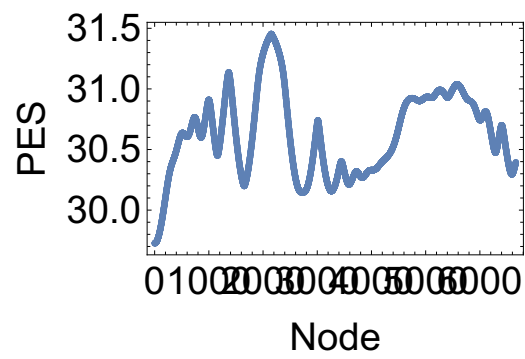
141.1656417188

```

start energy = 29.72688 detHess 90 777.78
0.3093127241 × 4.7928653504 × 8.2796529001
12.6772026860 × 17.1853581163 × 20.6978686584
25.1721232358 × 29.6857500777 × 33.2120405709
37.7130655533 × 42.2280440381 × 45.7597896694
50.2702636933 × 54.7855190624 × 58.3192020986
62.8330188584 × 67.3480014830 × 70.8821624077
75.3971282301 × 79.9109986388 × 83.4447101397
87.9599653951 × 92.4705917481 × 96.0024255959
100.5174222424 × 105.0188764926 × 108.5454038519
113.0590991657 × 117.5345668984 × 121.0476343563
125.5560849641 × 129.9571204106 × 133.4446352834
137.9295011177
SP node 594 energy = 31.4989116 detHess - 326.835086
3.9129867528 × 7.4044338830 × 11.7965247361
15.4925910045 × 19.4023683790 × 23.8372286010
27.3097407018 × 31.6040700011 × 36.0854347459
39.5677187300 × 44.0059839367 × 48.4679337150
51.9554818579 × 56.4359337232 × 60.8038901841
64.2745398462 × 68.7369946966 × 72.8303465491
76.3809419880 × 80.7635458825 × 84.3518445430
88.3940608226 × 92.8526629323 × 96.3266570633
100.6743308439 × 105.1648799390 × 108.6585065353
113.1149483625 × 117.5890021124 × 121.0873163160
125.5763968799 × 129.9782790631 × 133.4582519835
137.9364591169
node680 energy = 31.50025000 detHess 231.023526
3.9114788108 × 7.4058683790 × 11.8015241155
15.5047535947 × 19.4097970694 × 23.8462310403
27.3228028955 × 31.6136798510 × 36.1010237371
39.5887400206 × 44.0260585351 × 48.5071244683
52.0057285844 × 56.4900104022 × 60.9156684888
64.4003825007 × 68.8850939431 × 73.1418819634
76.6245961090 × 81.0485803848 × 84.8811366692
88.6555906720 × 93.0673499886 × 96.5543397255
100.7826478110 × 105.2599900837 × 108.7374707345
113.1534555688 × 117.6255309893 × 121.1145221296
125.5902248745 × 129.9925124593 × 133.4674702493
137.9411674042

```

NT34 PULL and PUSH start at gMin stepmax 1 eps10⁻¹¹



```

eps = E - 011 pred step 0.0075
start energy = 29.726842 detHess 91 060.91 ok minimum
0.3021918801 × 4.7868114594 × 8.2741990217
12.6745869008 × 17.1829799808 × 20.6959563571
25.1711938253 × 29.6848744256 × 33.2113682345
37.7127355013 × 42.2277260107 × 45.7595552253
50.2701471999 × 54.7854039021 × 58.3191249419
62.8329802944 × 67.3479628700 × 70.8821460618
75.3971223769 × 79.9109973827 × 83.4447290141
87.9599855413 × 92.4706333238 × 96.0024954161
100.5174922956 × 105.0190169620 × 108.5455993835
113.0593049278 × 117.5349890297 × 121.0481757003
125.5566755417 × 129.9583490093 × 133.4460167359
137.9311171953
SP node2708 energy = 30.14735845 detHess - 511.53662
0.8273453584, 5.7547168532, 10.1778760174,
13.9171327827, 18.6322802160, 23.1318574619,
26.7225053315, 31.3129733541, 35.8006699529,
39.3415638881, 43.8798920195, 48.3159938551,
51.8229465609, 56.3298110548, 60.6195616199,
64.1081097823, 68.5535947267, 72.4666704167,
76.1712475724, 80.5741283822, 84.0825219542,
88.2655582919, 92.7450360855, 96.2268269506,
100.6264359578, 105.1213711557, 108.6237345340,
113.0977249188, 117.5721046976, 121.0745786097,
125.5694710149, 129.9702672842, 133.4522791371,
137.9321665039
next point is again SP?
    node4751 energy = 30.9236945 detHess - 36 020.4148
SP4751 = {0.8312695463, 5.7612379360, 10.1926364966,
13.9294386814, 18.6447430613, 23.1566635049,
26.7495924605, 31.3414611869, 35.8589333472,
39.4124699878, 43.9558622770, 48.4728227583,
52.0142939542, 56.5399627489, 61.0569266329,
64.5946526167, 69.1140029723, 73.6323179212,
77.1696064111, 81.6868449385, 86.2095193851,
89.7491249966, 94.2659762503, 98.8010231425,
102.3487061818, 106.8660532282, 111.4352799807,
115.0086653268, 119.5246276260, 124.1841984604,
127.8479315065, 132.3293439756, 137.1839533737,
141.1730742195} end correctly moved

proof ' seldom' SP at 2708
Setxx = SP2708

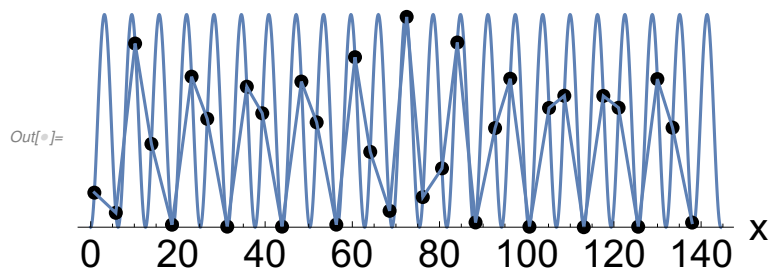
```

```
SetXX = {0.8298951589635579, 5.756545976130955, 10.180565910336638,
  13.918723547432649, 18.633117149012747, 23.13275789680411,
  26.723094281524943, 31.313239439574545, 35.80087787258329,
  39.341646754975876, 43.87984352845309, 48.31576582432948, 51.8226235455077,
  56.329388035362335, 60.61862586906689, 64.10722202133782,
  68.55249597295447, 72.46443137922259, 76.17005871719432, 80.57313750935492,
  84.08128755807749, 88.26499032796606, 92.7445916208072, 96.22647748705128,
  100.62631861695931, 105.1213690167663, 108.62385035045345,
  113.09792964457336, 117.57260305399913, 121.07525827621701,
  125.5702426258461, 129.97189947229825, 133.4541372906088, 137.9343564562487`}
```

ok is flat SP

Eigenvalues

```
Out[ ]= {4.29727, 4.28187, 4.2343, 4.18589, 4.11628, 4.03757, 3.94783,
  3.85127, 3.75908, 3.68815, 3.59927, 3.20988, 2.71793, 2.62424,
  2.49675, 2.34813, 2.19378, 2.03807, 1.88174, 1.75238, 1.62588,
  1.45991, 1.21666, 0.753455, 0.697587, 0.541954, 0.479181, 0.358496,
  0.296578, 0.215534, 0.167973, 0.128866, 0.0971963, -0.00343083}
```



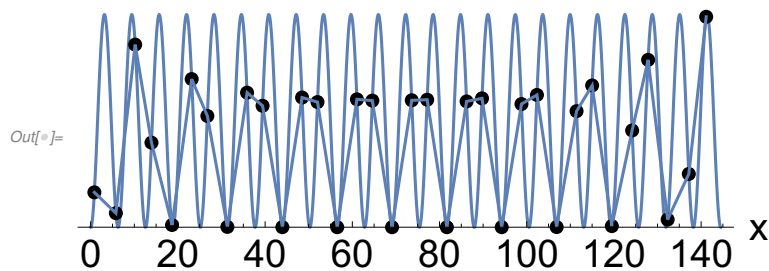
Setxx = SP4751

```
SetXX = {0.8337529313449289, 5.763002067001587, 10.195212053816304,
  13.9309752275722, 18.64555609693379, 23.157549140753577, 26.75020187377149,
  31.34176602504921, 35.859237624553494, 39.412692782202164,
  43.95597152399055, 48.47292768018619, 52.01437164164288, 56.539998941390756,
  61.05695752648754, 64.59467215476928, 69.11400699397676, 73.6323104483684,
  77.16958889335275, 81.68682073850856, 86.20946430242272, 89.74904926506942,
  94.26589591910786, 98.80085789361219, 102.34848300036478,
  106.86582637087184, 111.43482289372744, 115.00802240972854,
  119.5240130845395, 124.18300409600528, 127.8460508525638,
  132.32785762700948, 137.18148195130618, 141.16838308970213`}
```

Eigenvalues

ok it is strong SP1 with ordinary barrier

```
Out[ ]:= {4.31433, 4.29433, 4.2585, 4.20836, 4.14563, 4.07234, 3.99104, 3.90485, 3.81806,
  3.73959, 3.68847, 2.79844, 2.7394, 2.62868, 2.49127, 2.33986, 2.18155, 2.02116,
  1.86273, 1.71112, 1.57761, 1.49511, 1.21114, 0.749896, 0.648213, 0.541536,
  0.440721, -0.381162, 0.349807, 0.270982, 0.205908, 0.156246, 0.123983, 0.0998391}
```



schoenes Bild : x_34 geht gerade ueber seinen Top nach rechts

final node point in corrector

```
node6664 = {-0.0629838950, 4.5246520222, 8.1298588237,
  12.6972522544, 17.3951539780, 21.0998218837,
  25.5823958884, 30.4996244406, 34.6234970727,
  38.6814396789, 43.5711740614, 48.0612693594,
  51.7453548346, 56.4253095745, 60.9822187481,
  64.5777520062, 69.1579939332, 73.7811782056,
  77.4054317795, 81.9359595590, 86.7182978207,
  90.5528257711, 94.9129034835, 99.8901378038,
  104.2695134649, 108.0867616719, 112.8598811996,
  117.3977715746, 121.0193213333, 125.6385596995,
  130.2326542716, 133.8370188557, 138.3908290659,
  143.1047001364}
```

dNewtonStep length whould be 2.1220226919657126 node = 6664

Setxx = node6664

Shoulder only

```
SetXX = {0.34520191429397146, 4.872751169385698, 8.413853669111178,
  12.803467809871817, 17.42898712312513, 21.06762164139546,
  25.506948092921288, 30.314089786995208, 34.23291860705285,
  38.47753313392628, 43.42779121294485, 47.8541282367327, 51.61734754219343,
  56.35902624983509, 60.913432975253485, 64.52900802193686, 69.13762095591674,
  73.76935505692303, 77.403385749057, 81.94519935997779, 86.7481635536978,
  90.61382775278264, 94.95311954795825, 99.94116807862967, 104.37338439485733,
  108.16130593403402, 112.92464989624348, 117.5163342655355,
  121.15092845389348, 125.76580310028093, 130.4826650285743,
  134.20526589209018, 138.70072298441468, 143.64967343069517`}
```

ENERGY Shoulder 30.165653513079

Eigenvalues

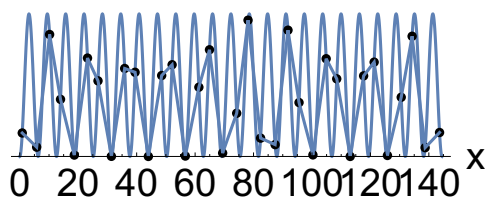
Out[*]= {4.33404, 4.3122, 4.26565, 4.21746, 4.15949, 4.07674, 3.99455, 3.93861, 3.85717, 3.7382, 3.27922, 2.92882, 2.84369, 2.68187, 2.54088, 2.38935, 2.21895, 2.05378, 1.90514, 1.76243, 1.59122, 1.47432, 1.3925, 1.16952, 0.537285, 0.457567, 0.44242, 0.317746, 0.228929, 0.190543, 0.138949, 0.118871, 0.0219876, -1.96926×10^{-14} }

min - Suche

SetXX = {0.8357972316337919, 5.766418936498196, 10.202969491318855, 13.937527264705011, 18.65222322242307, 23.170864829394027, 26.76500831008553, 31.357263301454363, 35.89088852840867, 39.45256737108646, 43.99761019747179, 48.5579656290075, 52.12765282293666, 56.6551900739951, 61.28904827433708, 64.923298092338, 69.42504451883664, 74.2318558395583, 78.11933950365997, 82.41501879638628, 87.38025339745893, 91.7938379099917, 95.57269854813379, 100.32148339260159, 104.86231538145114, 108.47486832268498, 113.08338119550868, 117.67793989593564, 121.28116962352424, 125.83048945792332, 130.54582019309197, 134.27551967052565, 138.73154705494437, 143.66828987243028`}

Eigenvalues

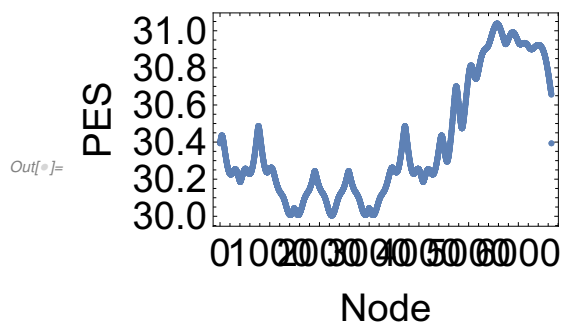
Out[*]= {4.32895, 4.29864, 4.26416, 4.21372, 4.14478, 4.07627, 3.98304, 3.90488, 3.82495, 3.71249, 3.6964, 2.90416, 2.76243, 2.66283, 2.52362, 2.36208, 2.20902, 2.03133, 1.88066, 1.7286, 1.55515, 1.49905, 1.20771, 1.19442, 0.637768, 0.539846, 0.453023, 0.335132, 0.286719, 0.199218, 0.153104, 0.110091, 0.101348, 0.010987}



it is asymmetric

NT34pushpullWeiter

new Predictor 0.0075, PULL and PUSH weiter rechnen
start at gMin stepmax 1 eps 10^{-11}



node1572 energy = 30.007023 detHess - 1355.8018
0.8342771638 \times 5.7660391907 \times 10.2033997530
13.9384596699 \times 18.6538422459 \times 23.1747581643
26.7696990323 \times 31.3624520314 \times 35.9017559998

39.4666149778 × 44.0121897012 × 48.5876525456
 52.1688374799 × 56.6952333325 × 61.3676707556
 65.0457849391 × 69.5241193531 × 74.4002206189
 78.4359304939 × 82.5753395570 × 87.4942893215
 91.9600803274 × 95.6720262725 × 100.3732543078
 104.9174244940 × 108.5142401336 × 113.1027101997
 117.6965549191 × 121.2967954274 × 125.8379503904
 130.5524694130 × 134.2825014934 × 138.7340450007
 143.6684930542

node2248 energy = 30.13186057 detHess 20.989

1.1582177101 × 5.9697889525 × 10.4730686416
 14.1097768794 × 18.7461102587 × 23.2791822222
 26.8519641892 × 31.4137520098 × 35.9733653049
 39.5449591646 × 44.0789650851 × 48.7094885588
 52.3401207290 × 56.8464880836 × 61.6462930341
 65.5193870625 × 69.8310982700 × 74.7992278705
 79.2035432244 × 82.9918008677 × 87.7463459146
 92.2843707685 × 95.8984819451 × 100.5094035641
 105.0987654784 × 108.6985613879 × 113.2495825831
 117.9522634744 × 121.6650856050 × 126.1338078411
 131.0555070957 × 135.1992639837 × 139.2324671393
 144.1084304211

node2924 energy = 30.00702134 detHess - 1349.1808

0.8409356425 × 5.7765885942 × 10.2270368261
 13.9585569413 × 18.6741690789 × 23.2152918597
 26.8158975553 × 31.4101985322 × 35.9987715326
 39.5957233830 × 44.1400660638 × 48.8415241342
 52.5537427393 × 57.0194376907 × 61.9387058420
 66.0789242428 × 70.1138594826 × 74.9896293309
 79.4680788452 × 83.1459473346 × 87.8181771214
 92.3445121333 × 95.9256075831 × 100.5009816107
 105.0463767981 × 108.6111089168 × 113.1503754309
 117.7426570034 × 121.3371867519 × 125.8581885753
 130.5724491492 × 134.3059252966 × 138.7444994033
 143.6751058380

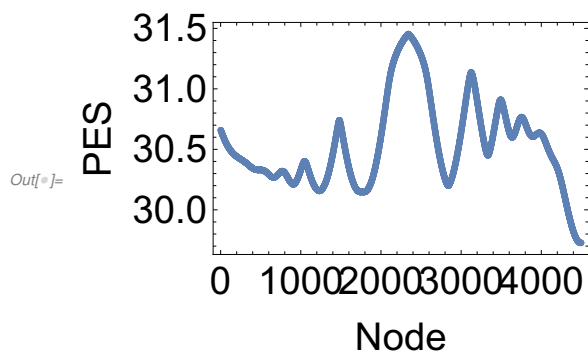
node3081 energy = 30.32658877 detHess - 180.6990

1.3303961809 × 6.0738540156 × 10.6095055434
 14.2187588814 × 18.8246868267 × 23.4057481811
 26.9989803697 × 31.5488873174 × 36.2313637691
 39.9191446449 × 44.4034718731 × 49.2966323616
 53.3655569959 × 57.4759878631 × 62.3864347668
 66.8660456696 × 70.5669498522 × 75.2607970751
 79.8176496598 × 83.4171086305 × 88.0030030807
 92.6272969119 × 96.2528242407 × 100.7855386015
 105.5700859591 × 109.4075370351 × 113.7661449976
 118.7448053762 × 123.1297123866 × 126.9437205992
 131.7157488434 × 136.2586871676 × 139.8807953496
 144.4997114583

SP node6404 energy = 30.923696376 detHess - 36 327.72

$3.3473880911 \times 7.3331026954 \times 12.1861998167$
 $16.6682173618 \times 20.3308946627 \times 24.9895769513$
 $29.5055830023 \times 33.0786812444 \times 37.6475556904$
 $42.1648968045 \times 45.7124903638 \times 50.2474080585$
 $54.7642523254 \times 58.3038257128 \times 62.8264536673$
 $67.3436822384 \times 70.8809545256 \times 75.3992522677$
 $79.9185785930 \times 83.4562864021 \times 87.9732420588$
 $92.4988453683 \times 96.0402732611 \times 100.5572282188$
 $105.1004434630 \times 108.6538526687 \times 113.1713290452$
 $117.7627314853 \times 121.3552378940 \times 125.8672726937$
 $130.5814710220 \times 134.3166836206 \times 138.7493236948$
 143.6781903411

NT34pushpullWeiter2

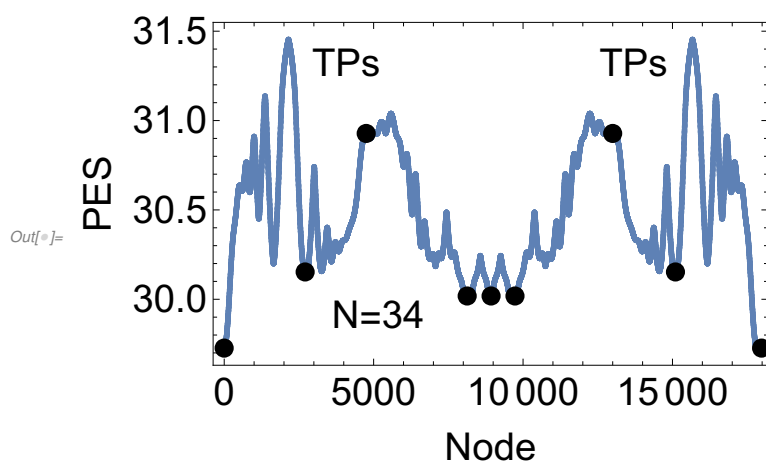


node1747 energy = 30.1473351 detHess 514.3388

6.5815317508 × 11.0606673775 × 14.5419200141
 18.9423725843 × 23.4355086069 × 26.9366267151
 31.4107023173 × 35.8795537246 × 39.3791870263
 43.8728553991 × 48.2573003487 × 51.7358832012
 56.2094306955 × 60.3502104338 × 63.8779125650
 68.2710705161 × 71.9169428085 × 75.8960083808
 80.3525542732 × 83.8382252736 × 88.1570449477
 92.6671296621 × 96.1772620206 × 100.6237541571
 105.1629025617 × 108.7052843106 × 113.1967961708
 117.7876048871 × 121.3786574312 × 125.8797817256
 130.5953042814 × 134.3347569648 × 138.7585708854
 143.6866183567

min node4494 energy = 29.7268601 detHess 91 058.125

6.5880717998 × 11.0722944894 × 14.5594454104
 18.9587617553 × 23.4670671550 × 26.9798675575
 31.4547316390 × 35.9683910856 × 39.4948109170
 43.9960465699 × 48.5110312117 × 52.0428330583
 56.5533786154 × 61.0686350086 × 64.6023471977
 69.1161864766 × 73.6311738541 × 77.1653569845
 81.6803283413 × 86.1942190461 × 89.7279595216
 94.2432162256 × 98.7539095618 × 102.2857989648
 106.8008016408 × 111.3024561260 × 114.8291121265
 119.3428400169 × 123.8188959465 × 127.3322571566
 131.8408482378 × 136.2435940336 × 139.7314954714
 144.2169984966

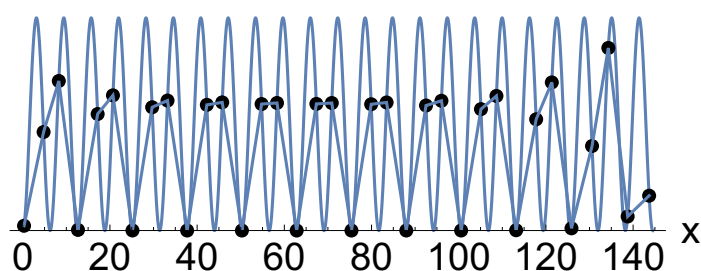


```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ###
```

```
N = 35 a_o minimum
```

```
ENERGY 30.67012291657261
```

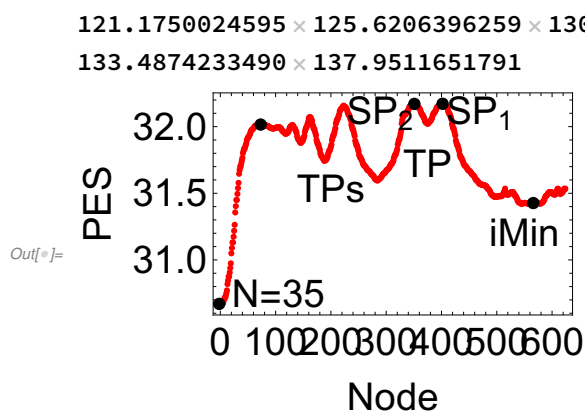
```
SetXX = {0.3005860662533404, 4.785456457974732, 8.272994950596479,
  12.674024461161201, 17.182500219263957, 20.695605172589538,
  25.171066515531884, 29.6848437784759, 33.21143934385268, 37.71289252311042,
  42.228126255743454, 45.76012619986035, 50.27077113148296, 54.78670493224853,
  58.32085563996991, 62.83479567656017, 67.35167849362705, 70.88704454685039,
  75.40223604677355, 79.92143998468183, 83.45848385034326, 87.97432767663757,
  92.49990470601203, 96.04111921520708, 100.55767305150772, 105.1009319048643,
  108.6543156163898, 113.17163835416592, 117.7631957509579,
  121.3558355214227, 125.86776743975969, 130.5823472652749,
  134.31812161311387, 138.7502915732682, 143.6795278309559` }
```



```
start energy 30.67012429558
```

```
0.2910550124 × 4.7773345433 × 8.2657215617
12.6705345217 × 17.1793237302 × 20.6930456698
25.1698257426 × 29.6836823594 × 33.2105268367
37.7124493611 × 42.2277091967 × 45.7597903342
50.2706069747 × 54.7865481245 × 58.3207134043
62.8347184774 × 67.3515889128 × 70.8869369584
75.4021550065 × 79.9213043497 × 83.4582962647
87.9741485471 × 92.4995550460 × 96.0406394753
100.5571892712 × 105.0999608302 × 108.6529785116
113.1703069086 × 117.7605428880 × 121.3519781291
125.8642206202 × 130.5756376044 × 134.3068970701
138.7425694811 × 143.6685931963
SP node73 energy = 32.015554852 detHess - 13 460.5
0.3004547039 × 4.7853154378 × 8.2728341242
12.6739090595 × 17.1823152880 × 20.6953686644
25.1708427816 × 29.6844092334 × 33.2108635226
37.7123032838 × 42.2269341033 × 45.7585490635
50.2691321647 × 54.7833649651 × 58.3164545857
62.8302042418 × 67.3423050687 × 70.8747259746
75.3893599060 × 79.8951301735 × 83.4240270983
87.9381989421 × 92.4259784926 × 95.9450946982
100.4562180755 × 104.8926641970 × 108.3899743247
112.8872718132 × 117.1760470860 × 120.6589668440
125.0994557526 × 129.0051621066 × 132.7123330975
137.1123596155 × 140.6132826369
SP2 ? node351 energy = 32.17151568 detHess 646.98
```

0.3018795375 × 4.7814479885 × 8.2634000652
 12.6627046283 × 17.1581942741 × 20.6609431185
 25.1348893167 × 29.6109836013 × 33.1143651923
 37.6096115555 × 42.0154770707 × 45.4987404535
 49.9805270744 × 54.1811990615 × 57.6827811099
 62.0905226906 × 65.8229945121 × 69.7053505975
 74.1443271137 × 77.6330975415 × 81.9093536390
 86.4115855505 × 89.9139756567 × 94.3455543103
 98.8747519549 × 102.4075953827 × 106.8940349444
 111.4602742906 × 115.0287083528 × 119.5328359982
 124.1886905386 × 127.8491285466 × 132.3265556830
 137.1745914522 × 141.1524877298
 SP1 node 402 energy = 32.17049006 detHess - 1118.72
 0.2821615710 × 4.7633929247 × 8.2459246978
 12.6526250548 × 17.1454729389 × 20.6471903468
 25.1232901239 × 29.5899389367 × 33.0889727192
 37.5827835380 × 41.9605282387 × 45.4382493036
 49.9093830215 × 54.0318957021 × 57.5694566129
 61.9595381370 × 65.5838000418 × 69.5879226278
 74.0475011167 × 77.5311982549 × 81.8609914431
 86.3694033849 × 89.8781128599 × 94.3286656790
 98.8600163979 × 102.3963781568 × 106.8896533658
 111.4583600018 × 115.0293899394 × 119.5358727698
 124.1970834040 × 127.8637152012 × 132.3388380717
 137.1959490833 × 141.1936434102
 iMin ? 546 energy = 31.42646767 detHess 173.37553
 0.2876954203 × 4.7530491895 × 8.2192294711
 12.6194450199 × 17.0727100603 × 20.5471283061
 25.0135212248 × 29.3609763595 × 32.8233623794
 37.2724347233 × 41.3076589448 × 44.8927142946
 49.2675293359 × 52.8019810876 × 56.9052722475
 61.3576577624 × 64.8147055282 × 69.1880525864
 73.6343489952 × 77.0992271973 × 81.5556404137
 85.8866163507 × 89.3434753806 × 93.7819751333
 97.7713331733 × 101.3879504285 × 105.7604400424
 109.2636663272 × 113.4050299504 × 117.8492557210
 121.2942627483 × 125.6810380380 × 130.0851443543
 133.5312791029 × 137.9773214909
 to node572 energy = 31.43045332 detHess - 253.807
 0.2731318932 × 4.7320284758 × 8.1911179071
 12.5939131528 × 17.0242474549 × 20.4867955160
 24.9471370351 × 29.2229381705 × 32.6861364551
 37.1044977692 × 40.9626699747 × 44.6991788618
 49.0927248718 × 52.5644479096 × 56.7825650548
 61.2324526429 × 64.6827493006 × 69.0940737832
 73.4844352058 × 76.9330440262 × 81.3810057806
 85.5330621485 × 89.0332388645 × 93.4099645014
 97.0435071300 × 101.0160604630 × 105.4549066823
 108.9160468596 × 113.2394373415 × 117.7044518765



```
## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ==
```

```
N = 35 SP2 indeet
```

```
SetXX = {0.2959541322160949, 4.776397057209328, 8.25888793380375,
12.660518266654469, 17.156157292095383, 20.659302533220124,
25.134034560384077, 29.610059611536062, 33.11358593149831,
37.609074720728835, 42.0146465320512, 45.49793366468268, 49.9796960632269,
54.17954178160748, 57.68147352688692, 62.08900277749841,
65.82013200662736, 69.70395584437537, 74.1432314022205,
77.63195235431792, 81.9088560225784, 86.4112469160073, 89.91378686020907,
94.34558247511362, 98.87502394971726, 102.40808711892437,
106.8945976064611, 111.46146852362524, 115.03045572403325,
119.5345186214433, 124.19197143571493, 127.85432700508895,
132.33066317173876, 137.18141991683262, 141.16542252388896`}
```

Eigenvalues

```
Out[*]= {4.30057, 4.28386, 4.24398, 4.19742, 4.13872, 4.06678, 3.99043,
3.90495, 3.81936, 3.73877, 3.59991, 3.21024, 2.75748, 2.63867,
2.55123, 2.39975, 2.26498, 2.11031, 1.97475, 1.81303, 1.7325, 1.56349,
1.45919, 0.755197, 0.711983, 0.551372, 0.502136, -0.380748, 0.375627,
0.318461, 0.233976, 0.186948, 0.140996, 0.121324, -0.00551145}
```

```
ENERGY SP2 32.1697809544
```

```
start at ao Min, stepmax = 1.0 eps 10^-10 normal conv
```

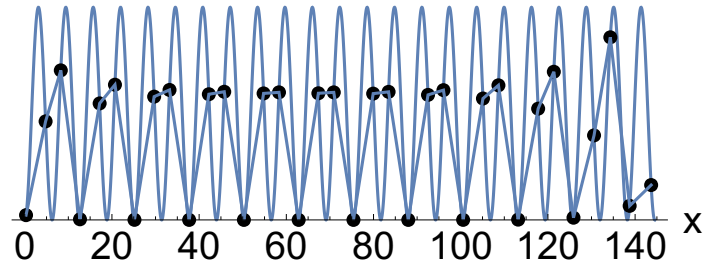
```
N = 35 global minimum
```

```
ENERGY 30.670122916572865
```

```
SetXX = {0.3005857200937027, 4.785456105279612, 8.272994659298401,
12.674024242647356, 17.182499898723368, 20.69560489136664,
25.171066374910637, 29.68484394492806, 33.211440020992704,
37.71289297338945, 42.22812710673596, 45.760126679543816,
50.27077158692502, 54.78670546626585, 58.320856258440614,
62.834796260573235, 67.35167913335886, 70.88704473350091, 75.40223641810142,
79.92144073069264, 83.45848444800359, 87.97432823843725, 92.49990583441296,
96.04112057730637, 100.55767398461697, 105.10093258208346,
108.6543160508243, 113.17163873967982, 117.76319615768696,
121.35583574441227, 125.86776755902709, 130.5823473985709,
134.31812162879967, 138.75029151336315, 143.67952784449912`}
```


Eigenvalues

```
{4.3131, 4.29151, 4.2551, 4.20476, 4.14152, 4.06681, 3.98282,
 3.89317, 3.80453, 3.73018, 3.68788, 3.2174, 2.77941, 2.69441,
 2.56984, 2.42479, 2.26903, 2.10841, 1.94742, 1.79078, 1.64594,
 1.53031, 1.43771, 1.21118, 0.771614, 0.688168, 0.58843, 0.489508,
 0.39793, 0.316688, 0.247444, 0.191317, 0.149241, 0.122175, 0.0998218}
```



```
node116 energy 30.818233, detHess 1601.22683
first flat iMin whatever it means between glob Minimums
node116 = {0.2976206047, 4.7834724225, 8.2718496045,
12.6741830082, 17.1841200674, 20.6985321050,
25.1745009957, 29.6922175170, 33.2216024213,
37.7235297038, 42.2498724206, 45.7892485971,
50.3008695046, 54.8478700741, 58.4033089267,
62.9187335748, 67.5209294682, 71.1233970876,
75.6316519590, 80.3712210017, 84.1445566362,
88.5454754177, 93.4951549449, 97.7612776256,
101.6640091086, 106.4724474233, 110.9457938087,
114.5830862702, 119.2167645349, 123.6874174024,
127.2391620047, 131.7908957514, 136.1872657129,
139.6929816334, 144.1928829150}
```

ENERGY 30.818219649416

```
{0.30108, 4.78642, 8.2745, 12.6755, 17.1853, 20.6995, 25.175, 29.6927, 33.222,
 37.7238, 42.2502, 45.7895, 50.3011, 54.8483, 58.4038, 62.9192, 67.5219, 71.1248,
 75.6329, 80.3736, 84.1487, 88.5481, 93.4985, 97.7677, 101.668, 106.475,
 110.949, 114.585, 119.218, 123.689, 127.241, 131.793, 136.19, 139.696, 144.196}
```

Eigenvalues

```
{4.32527, 4.29532, 4.25792, 4.21132, 4.14599, 4.07714, 4.00068,
 3.89909, 3.85341, 3.75839, 3.241, 3.21819, 2.8809, 2.71997, 2.5907,
 2.44708, 2.28458, 2.13188, 1.97821, 1.79761, 1.69512, 1.54661,
 1.43364, 1.41136, 0.724872, 0.579141, 0.562023, 0.429551, 0.340039,
 0.293155, 0.21552, 0.169288, 0.137259, 0.114817, 0.00410034}
```

```

stat points by node374 energy30 .82337 ? SP : detHess - 5646.25501
? New Min node527 energy30 .671050 detHess 76 424
→ is the mirror image
node374 = {0.2747194244, 4.7702164315, 8.2673796892,
12.6823588848, 17.2130944072, 20.7459012299,
25.2263623612, 29.8003080820, 33.3752288276,
37.8757028715, 42.5518875429, 46.2375312316,
50.6985353241, 55.5794611674, 59.6350380452,
63.7458208898, 68.6494208026, 73.1037813005,
76.8082023309, 81.5001236488, 86.0117136284,
89.5952938524, 94.1772283664, 98.6886619460,
102.2366135886, 106.7756296460, 111.2761314092,
114.8077385890, 119.3297847834, 123.8011109991,
127.3145147951, 131.8250284303, 136.2139403791,
139.6994427416, 144.1800465096}
N = 35
Setxx = node374

ENERGY 30.82093804387823
{0.305419, 4.7949, 8.28779, 12.688, 17.2097, 20.7337, 25.209, 29.7606, 33.3157,
37.8172, 42.4364, 46.056, 50.5518, 55.3299, 59.1694, 63.5065, 68.4682, 72.8273,
76.6462, 81.4134, 85.9159, 89.5304, 94.1448, 98.6566, 102.214, 106.765, 111.267,
114.803, 119.329, 123.805, 127.322, 131.835, 136.235, 139.725, 144.211}

Eigenvalues
{4.32678, 4.2935, 4.26079, 4.20888, 4.14906, 4.07636, 3.99535,
3.92188, 3.81782, 3.77989, 3.22482, 3.21992, 2.88952, 2.71673,
2.59424, 2.4428, 2.28983, 2.12923, 1.96813, 1.82846, 1.6489, 1.56573,
1.43065, 1.42229, 0.694623, 0.649307, 0.514086, 0.438699, 0.355804,
0.277591, 0.225357, 0.168028, 0.138574, 0.114634, 0.0119121}

Minimization geht zu next iMin ok

NMinimize[G2G2G2, SetFin]
goes to the correct SP_1

SetXX = {0.3082807286192931, 4.800491799944371, 8.296581414896826,
12.69631228747772, 17.225619467744806, 20.756338252331105,
25.23114271980719, 29.80418995403394, 33.37807512345453, 37.87635439336483,
42.55094966000304, 46.235252169771215, 50.69576821669575,
55.573414794404584, 59.62321755163033, 63.740012963275426,
68.64518141983558, 73.09759112634423, 76.80471722927223,
81.49837596718925, 86.01002193608042, 89.59441049637624, 94.1770578897115,
98.6890425034924, 102.23755719406614, 106.77686577448706,
111.27889854511336, 114.81143788057457, 119.33372646870077,
123.80923776495064, 127.32471489229023, 131.83612563799923,
136.23699693086158, 139.72571278430942, 144.21160543179275`}

```

Eigenvalues

```
{4.32532, 4.29422, 4.25939, 4.2093, 4.1492, 4.07309, 4.00202,
 3.91155, 3.83202, 3.77189, 3.22902, 3.21909, 2.88426, 2.71934,
 2.59273, 2.4431, 2.29277, 2.12279, 1.98109, 1.81501, 1.66536,
 1.56053, 1.43171, 1.41918, 0.706555, 0.623602, 0.535073, 0.410873,
 0.371995, 0.27072, 0.225074, 0.17108, 0.13591, 0.118411, -0.0121774}
```

```
ENERGY SP 30.822201380039246`
```

```
SP ok
```

```
node527 = {0.8016368303, 5.7397838623, 10.1608801449,
13.9105717702, 18.6347004609, 23.1456229369,
26.7419627655, 31.3375644933, 35.8548843497,
39.4093540962, 43.9541170403, 48.4707036037,
52.0122695487, 56.5383890551, 61.0542300330,
64.5913835165, 69.1107795224, 73.6259166847,
77.1612885112, 81.6782336213, 86.1920033646,
89.7260646398, 94.2420026370, 98.7521636956,
102.2838798722, 106.7990582587, 111.2991452544,
114.8249749314, 119.3385300898, 123.8101068320,
127.3214056879, 131.8289317394, 136.2187713256,
139.7040723076, 144.1846924045}
```

```
ENERGY 30.670122916571916
```

```
{0.833734, 5.76297, 10.1951, 13.9309, 18.6455, 23.1574, 26.7501, 31.3416, 35.8589,
 39.4123, 43.9556, 48.4721, 52.0134, 56.5389, 61.0548, 64.5918, 69.111, 73.6262,
 77.1616, 81.6785, 86.1924, 89.7266, 94.2425, 98.7531, 102.285, 106.8, 111.302,
 114.828, 119.342, 123.818, 127.331, 131.839, 136.24, 139.728, 144.213}
```

Eigenvalues

```
{4.3131, 4.29151, 4.2551, 4.20476, 4.14152, 4.06681, 3.98282,
 3.89317, 3.80453, 3.73018, 3.68788, 3.2174, 2.77941, 2.69441,
 2.56984, 2.42479, 2.26903, 2.10841, 1.94742, 1.79078, 1.64594,
 1.53031, 1.43771, 1.21118, 0.771614, 0.688168, 0.58843, 0.489508,
 0.39793, 0.316688, 0.247444, 0.191317, 0.149241, 0.122175, 0.0998217}
```

```
next iMin
```

```
NMinimize[G2G2G2, SetFin]
```

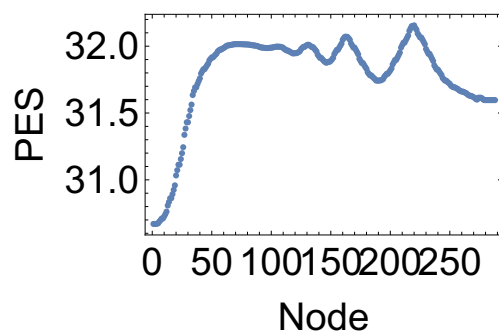
```
{0.833734, 5.76297, 10.1951, 13.9309, 18.6455, 23.1574, 26.7501, 31.3416, 35.8589,
 39.4123, 43.9556, 48.4721, 52.0134, 56.5389, 61.0548, 64.5918, 69.111, 73.6262,
 77.1616, 81.6785, 86.1924, 89.7266, 94.2425, 98.7531, 102.285, 106.8, 111.302,
 114.828, 119.342, 123.818, 127.331, 131.839, 136.24, 139.728, 144.213}
```

```
again iMin but not the SP
```

```

next min node579 ? energy = 30.674477 detHess 93 720.6
node579 = {0.9033937465, 5.8107483958, 10.2630452907,
13.9718565408, 18.6670351172, 23.1807045952,
26.7661692877, 31.3496736418, 35.8669735491,
39.4182289965, 43.9585052111, 48.4749917302,
52.0155141098, 56.5400168173, 61.0558686853,
64.5926978629, 69.1115221249, 73.6268301401,
77.1621904002, 81.6789512063, 86.1932542277,
89.7275988407, 94.2435282557, 98.7552063314,
102.2878157346, 106.8031668800, 111.3075349041,
114.8357886313, 119.3500209103, 123.8337579895,
127.3508870898, 131.8612514572, 136.2860804481,
139.7797427991, 144.2731820409}
similar iMin like above

```



```

node 73 seems to be SP energy = 32.015404 detHess - 13 889.89
node73 = {3.8882696971, 7.3913776462, 11.7893790207,
15.4862428720, 19.4030149527, 23.8454200383,
27.3277358603, 31.6214836109, 36.1193439001,
39.6172444341, 44.0554277363, 48.5666764572,
52.0861072342, 56.5744928609, 61.0887007134,
64.6177251330, 69.1237097862, 73.6383657380,
77.1708406660, 81.6830188397, 86.1968068590,
89.7299349646, 94.2441989301, 98.7548822258,
102.2865628709, 106.8012162370, 111.3029359787,
114.8295509347, 119.3431660950, 123.8194352006,
127.3328660151, 131.8414630355, 136.2448268408,
139.7328541554, 144.2185690744}
Setxx = node73

```

```
NMinimize[G2G2G2, SetFin]
```

```

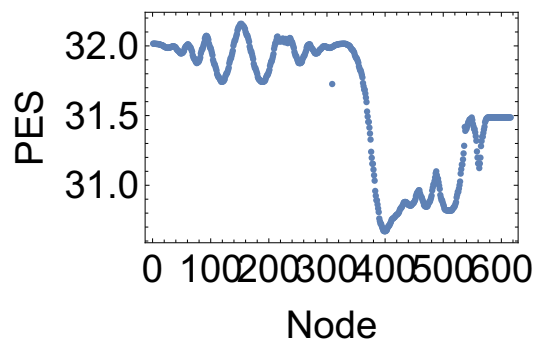
{3.92037, 7.41456, 11.8236, 15.5066, 19.4138, 23.8572, 27.3358, 31.6255, 36.1234,
39.6202, 44.0569, 48.5681, 52.0872, 56.575, 61.0892, 64.6182, 69.124, 73.6387,
77.1711, 81.6833, 86.1972, 89.7304, 94.2447, 98.7559, 102.288, 106.803, 111.306,
114.833, 119.347, 123.827, 127.342, 131.852, 136.266, 139.757, 144.247}

```

Eigenvalues

gibt schoenen SP_1 o.k.

SP ENERGY 32.0164294415526 start hier



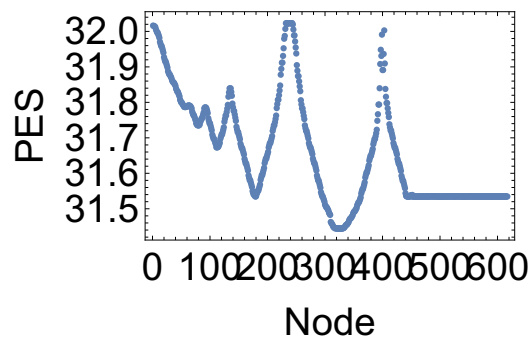
node331 is again SP but NT is turned?

node402 next min energy 30.6701237

detHess 100 326.80 it is known Min bevor Mountains

node401 = {0.8346817315 × 5.7636425995 × 10.1961202285 ×
 13.9314996180 × 18.6458039289 × 23.1577631135 ×
 26.7502978179 × 31.3417394604 × 35.8590620595 ×
 39.4124149043 × 43.9556308370 × 48.4721836168 ×
 52.0133881251 × 56.5389497288 × 61.0547934497 ×
 64.5918341320 × 69.1110326965 × 73.6262255891 ×
 77.1615913660 × 81.6784725098 × 86.1924171743 ×
 89.7265705175 × 94.2425045797 × 98.7531636383 ×
 102.2851718219 × 106.8004073827 × 111.3019005368 ×
 114.8285190314 × 119.3423030513 × 123.8178785889 ×
 127.3310374092 × 131.8395403496 × 136.2408982604 ×
 139.7285087393 × 144.2135020614}

Start SP dir - EV



```
stat point node328 energy = 31.443986316 detHess 40.18
```

? BBP point crossed ? sieht aus wie hinter dem Gebirge ?

aber compressed Vorderer Teil : evt richtiges iMin

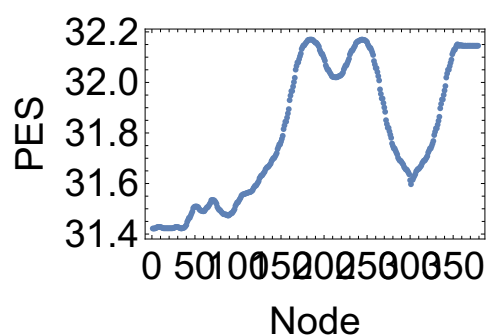
```
node328 = {6.4138346512, 10.7699208557, 14.1694903624,
18.5791504932, 22.7347400973, 26.2187271933,
30.5906741666, 34.2305364755, 38.1926321265,
42.6291492548, 46.0897332663, 50.4099386596,
54.8742311347, 58.3439750515, 62.7886564861,
67.1901793603, 70.6537458777, 75.1168038480,
79.3021464127, 82.7968833046, 87.1897408030,
90.8829877214, 94.7975857771, 99.2347060138,
102.7092756957, 107.0049148438, 111.4901637312,
114.9760741607, 119.4149438781, 123.8882298464,
127.3823897378, 131.8656342261, 136.2677108814,
139.7454763415, 144.2217077950}
Setxx = node328
```

```
ENERGY 31.42196949947214
```

```
{6.54274, 10.9882, 14.4337, 18.8355, 23.2233, 26.6678, 31.1118, 35.2563, 38.7575,
43.1303, 46.7504, 50.7354, 55.1732, 58.6301, 62.9594, 67.4159, 70.8806, 75.3264,
79.7005, 83.1575, 87.61, 91.7153, 95.2485, 99.6235, 103.211, 107.243, 111.692,
115.155, 119.501, 123.969, 127.443, 131.896, 136.299, 139.766, 144.232}
```

Eigenvalues

```
{4.28591, 4.26081, 4.23343, 4.1776, 4.11065, 4.0367, 3.9502,
3.85768, 3.76482, 3.62912, 3.57108, 3.18844, 3.15855, 2.63149,
2.52358, 2.4177, 2.27263, 2.12083, 1.97799, 1.86673, 1.73076, 1.53345,
1.49464, 0.791135, 0.705219, 0.662078, 0.515383, 0.412932, 0.343159,
0.271433, 0.206277, 0.162004, 0.134487, 0.0165619, 0.00928772}
```



```

node185 next SP energy = 32.1696182
detHess - 1220.308 node 300 is TP or so not min
node185 = {6.5755392964, 11.0552829298, 14.5368085946,
18.9395347410, 23.4321183419, 26.9331175801,
31.4078788725, 35.8745925883, 39.3733216621,
43.8667083243, 48.2447633815, 51.7223377376,
56.1934278323, 60.3167026002, 63.8537111476,
68.2437986990, 71.8687585224, 75.8719381674,
80.3313126794, 83.8149427448, 88.1443706664,
92.6526081358, 96.1611426644, 100.6115727827,
105.1425235038, 108.6785533035, 113.1717893887,
117.7394105649, 121.3095027481, 125.8161293858,
130.4745897467, 134.1378967828, 138.6149608184,
143.4674765357, 147.4546737232}
Setxx = node185

SetXX = {6.579152764902046, 11.05960834922722, 14.542113413634631,
18.943741964737956, 23.439417366560367, 26.9425898802891, 31.4173251975523,
35.89345917601385, 39.39704537301758, 43.89256051622251, 48.298459413396486,
51.78183449140907, 56.26372784497373, 60.46452140456562, 63.96612704672391,
68.37396014565762, 72.10670948367243, 75.98881938351525, 80.42778519669675,
83.91662995988659, 88.19274640922755, 92.69504076424265, 96.19749815118001,
100.62901940613108, 105.15843810071306, 108.69145997547723,
113.17787323892063, 117.74473717468899, 121.31371204421599,
125.81773739946038, 130.4751856513333, 134.1375393536835,
138.6138577432257, 143.4646052098187, 147.44859854295865` }

ENERGY SP 32.169781038635

Eigenvalues -- it is 'flat' index 2
{4.300558349341938, 4.283886294224036, 4.243955719432981, 4.197441028450062,
4.138699415532092, 4.0667925118277335, 3.990422550009756, 3.9049495490374735,
3.819357093060233, 3.73876523228245, 3.599925160221427, 3.21025707304395,
2.757432783465831, 2.638749721565808, 2.551180599893129, 2.3997648847484276,
2.2649849029667966, 2.1102931869066515, 1.9747668152689872,
1.81307348854964, 1.7324381519682905, 1.563574429455612, 1.4591467977000274,
0.7552303582989364, 0.7119002600773849, 0.5514101591243596,
0.5020880344290348, -0.38074710346607166, 0.37560168181143494,
0.3184763412745055, 0.23394384513399036, 0.1869673825878077,
0.14098311265212082, 0.1213329937124054, -0.0056357402182793}

```

```

node306 = {6.8185062435, 11.2607035177, 14.7378421310,
19.0399349517, 23.5312588652, 27.0230535316,
31.4642358052, 35.9537085614, 39.4583862863,
43.9453547594, 48.3953892345, 51.8898786513,
56.3829334959, 60.7110114319, 64.1865810414,
68.6389067126, 72.6328822140, 76.2594017908,
80.6445440877, 84.1688632281, 88.3016708567,
92.7652096305, 96.2326345827, 100.6155572689,
105.0829715021, 108.5632190767, 113.0276182964,
117.4223567455, 120.8911885891, 125.3582133072,
129.5244747488, 133.0319706822, 137.4238075602,
141.0939339851, 145.0382399304}
Setxx = node306

```

ENERGY 31.421969499472176

```

{6.5643, 11.0305, 14.4973, 18.9, 23.3531, 26.8279, 31.295, 35.6415, 39.1041,
43.5531, 47.5859, 51.1729, 55.548, 59.0811, 63.1864, 67.6389, 71.0959, 75.47,
79.9158, 83.3805, 87.837, 92.1663, 95.6232, 100.061, 104.046, 107.666, 112.039,
115.54, 119.685, 124.129, 127.573, 131.961, 136.363, 139.808, 144.254}

```

Eigenvalues

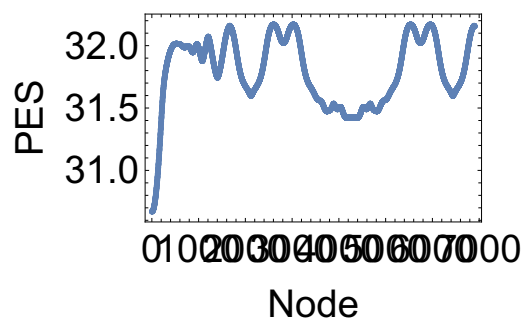
```

{4.28591, 4.26081, 4.23343, 4.1776, 4.11065, 4.0367, 3.9502,
3.85768, 3.76482, 3.62912, 3.57108, 3.18844, 3.15855, 2.63149,
2.52358, 2.4177, 2.27263, 2.12083, 1.97799, 1.86673, 1.73076, 1.53345,
1.49464, 0.791135, 0.705219, 0.662078, 0.515383, 0.412932, 0.343159,
0.271433, 0.206277, 0.162004, 0.134487, 0.0165619, 0.00928775}

```

In Sum by N = 35 hoert die Gutartigkeit auf, NTs arbeiten oft noch,
aber nicht immer, push and pull versagt global

Start a0 - Min mit PP = (1, 0, ..., 0, 1)
NT35D pred 0.01 direction PP



am 3. SP nach min : wieder SP1, vorher ist ein SP2,
der 1. SP ist im Vorgebirge?

SD von 1. SP aus : geht es zum iMin

dann sind die inneren SPs ueberfluessig

IRC final point ist iMin ok !

0.29888777152018992 × 4.7798607877833597 × 8.2683480508809488
12.662678683767620 × 17.173359406574580 × 20.672690398523077
25.160319343020852 × 29.640980995285350 × 33.166496548032171
37.649273994474974 × 42.122213745836312 × 45.610007530913855
50.121819612377294 × 54.452739449630208 × 57.937421956015768
62.380939482398539 × 66.412036424105196 × 69.999350018123423
74.374599391096041 × 77.876967984300038 × 82.000451229552894
86.419423751675211 × 89.847656159179166 × 94.216273082015547
98.564975563784600 × 101.98153643021240 × 106.39641915786042
110.39610069462050 × 113.97063443516203 × 118.30541033556598
121.76293557637109 × 125.90501474078599 × 130.28791600858386
133.67260771093498 × 138.04549651309429

start eps = 1.0 E - 010 energy 30.6701242955

detHess 82798.32 point in corrector

0.2993347707 × 4.7843912919 × 8.2720388472
12.6735658115 × 17.1820828095 × 20.6952692488
25.1709035818 × 29.6846910150 × 33.2113209155
37.7128348574 × 42.2280713876 × 45.7600835983
50.2707501220 × 54.7866842876 × 58.3208387219
62.8347860636 × 67.3516663939 × 70.8870318054
75.4022256997 × 79.9214215983 × 83.4584603835
87.9743042629 × 92.4998579558 × 96.0410569996
100.5576094140 × 105.1008031784 × 108.6541398512
113.1714628091 × 117.7628451843 × 121.3553259094
125.8672991781 × 130.5814619051 × 134.3166383105
138.7492739544 × 143.6780928960

SP node525 energy = 32.01534161 detHess - 14555.49

0.3027082810 × 4.7872336156 × 8.2745555107
12.6747348102 × 17.1830665854 × 20.6959713266
25.1711349357 × 29.6846828857 × 33.2110730374
37.7124038800 × 42.2270263887 × 45.7586143773
50.2691588844 × 54.7833798141 × 58.3164530540
62.8301881711 × 67.3422583835 × 70.8746564877
75.3892823206 × 79.8949668903 × 83.4238114638
87.9379692646 × 92.4255051318 × 95.9444940197
100.4555669903 × 104.8913133940 × 108.3883879897
112.8854578673 × 117.1722317368 × 120.6554149198
125.0951376076 × 128.9964339498 × 132.7077567075
137.1086279572 × 140.6087675473

goes back because minus steps are used

node2605 energy = 32.15693102 detHess 1122.56539

0.1535405696 × 4.6524902812 × 8.1532315807
12.6095319861 × 17.1089803645 × 20.6228065717

25.1162090752 × 29.5930801629 × 33.1015468522
 37.6034301083 × 42.0097773654 × 45.4957334006
 49.9800482940 × 54.1827879947 × 57.6852967669
 62.0950327272 × 65.8328259450 × 69.7107793379
 74.1498603285 × 77.6404674885 × 81.9140023884
 86.4180399784 × 89.9223685768 × 94.3527528243
 98.8879177590 × 102.4256911520 × 106.9114566380
 111.4943751141 × 115.0778107517 × 119.5784952200
 124.2758634294 × 127.9899165504 × 132.4319576412
 137.3402663115 × 141.4716129915

etwas relaxed

node3027 energy = 32.1696184 detHess - 1279.14759

0.2972590630 × 4.7762784517 × 8.2573369267
 12.6581451023 × 17.1505989988 × 20.6512541412
 25.1253699056 × 29.5921144082 × 33.0906964345
 37.5838787580 × 41.9620827595 × 45.4395863487
 49.9106553428 × 54.0342959825 × 57.5710397277
 61.9611306424 × 65.5864268305 × 69.5891524995
 74.0484289063 × 77.5320264057 × 81.8612786744
 86.3694324777 × 89.8778822188 × 94.3282534593
 98.8590118054 × 102.3948816261 × 106.8880988428
 111.4551973916 × 115.0248394377 × 119.5315341303
 124.1886688235 × 127.8503844878 × 132.3283696573
 137.1786476486 × 141.1607796839

node4159 energy = 31.42197613 detHess 225.717

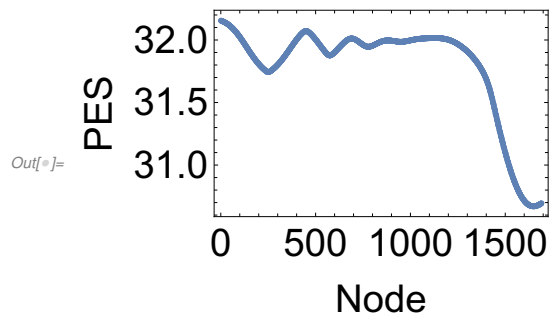
0.2786687389 × 4.7452059013 × 8.2122743371
 12.6158439785 × 17.0688668137 × 20.5438361925
 25.0111911366 × 29.3572950557 × 32.8200493407
 37.2689457721 × 41.3008204270 × 44.8886429218
 49.2637211253 × 52.7963779978 × 56.9024738905
 61.3550404947 × 64.8120202257 × 69.1863714410
 73.6319952844 × 77.0966548670 × 81.5531805322
 85.8818287615 × 89.3386952517 × 93.7762796678
 97.7596409032 × 101.3811361882 × 105.7540249157
 109.2544966677 × 113.4001388073 × 117.8439784577
 121.2884042725 × 125.6765523494 × 130.0775464253
 133.5227751906 × 137.9679938017

node4251 energy = 31.4227919 detHess - 42.0613

0.2793853461 × 4.7430507489 × 8.2071837347
 12.6095879228 × 17.0551959676 × 20.5256904455
 24.9906420371 × 29.3139721153 × 32.7750809847
 37.2138774312 × 41.1862580334 × 44.8199210808
 49.1966392881 × 52.6967129555 × 56.8488951004
 61.2968146788 × 64.7453733398 × 69.1357748510
 73.5469113608 × 76.9971348713 × 81.4469634084
 85.6644880806 × 89.1363783090 × 93.5297137220
 97.2651197616 × 101.1244589588 × 105.5430591212
 109.0062354823 × 113.2825407087 × 117.7429944780
 121.2056728883 × 125.6361777411 × 130.0391570258

133.4983614582 × 137.9573794487
 node4402 energy = 31.42197469 detHess 234.160
 0.2573174897 × 4.7029614556 × 8.1486421036
 12.5512283597 × 16.9386729359 × 20.3833913527
 24.8274269073 × 28.9708694808 × 32.4727478513
 36.8454233316 × 40.4643891613 × 44.4508513038
 48.8889102009 × 52.3457713560 × 56.6756246823
 61.1320941824 × 64.5968676027 × 69.0428400603
 73.4166768460 × 76.8736917239 × 81.3261668327
 85.4308242358 × 88.9643999699 × 93.3393421257
 96.9257398577 × 100.9593377160 × 105.4083269625
 108.8708923699 × 113.2176916002 × 117.6845568116
 121.1592443848 × 125.6123933466 × 130.0142510840
 133.4808621571 × 137.9467978748
 5536 energy = 32.16961378 detHess - 1283.6998
 - 2.9438809677 × 1.0444808800 × 5.8975097465
 10.3743530993 × 14.0380240259 × 18.6967976177
 23.2034053455 × 26.7735945313 × 31.3413477946
 35.8345909246 × 39.3706563350 × 43.9016563265
 48.3521026425 × 51.8606569199 × 56.3689150209
 60.6983865519 × 64.1820227558 × 68.6414209225
 72.6447093990 × 76.2695860229 × 80.6596714161
 84.1967378269 × 88.3199291259 × 92.7910256897
 96.2686148369 × 100.6466371236 × 105.1400740471
 108.6388369189 × 113.1055436031 × 117.5804582919
 121.0815374368 × 125.5741515794 × 129.9773287632
 133.4589612358 × 137.9388699457
 node5959 energy = 32.16977575 detHess 1220.859
 - 2.9291489369 × 1.0519213753 × 5.9013730890
 10.3782219142 × 14.0396550003 × 18.6963409169
 23.2004103188 × 26.7691230962 × 31.3356955238
 35.8221226547 × 39.3550587013 × 43.8843751850
 48.3159259233 × 51.8183515607 × 56.3206170598
 60.5968031871 × 64.0856112123 × 68.5245830732
 72.4068146460 × 76.1394262206 × 80.5472144584
 84.0488066712 × 88.2495421256 × 92.7313855637
 96.2147058283 × 100.6205897520 × 105.1159787118
 108.6194665895 × 113.0955814624 × 117.5699422578
 121.0729116080 × 125.5684988230 × 129.9690204721
 133.4512564945 × 137.9312870481

FKmketen35Dpr0p01PPweiter



Join[FKmketen35Dpr0p01PP, FKmketen35Dpr0p01PPweiter]

