NOTES ON LOCALIZATION/DIAGONALIZATION PROBLEM

Dear John,

Here is a very 'high level' description of the localization problem:

[1] 1D chain of j=1,2,...N identical masses connected by identical springs k.

[2] Diagonalize this matrix (note the periodic boundary conditions):

```
2k   -k   0   0   [...]  0   -k
-k   2k  -k   0   [...]  0    0
 0   -k  2k   0   [...]  0    0
 [...]
 0    0   0   0   [...] 2k   -k
-k    0   0   0   [...] -k   2k
```

[3] Eigenvectors are all 'extended'. Visualize by plotting squares of components vs mass number j.

[4] Or, show extended by computing 'participation ratios' P_n. For eigenvector V_n with components V_n(j)

P_n = sum(j) 1/V_n(j)^4

P is big (order N) for delocalized state, and small (order 1) for localized state. [4] is more convenient than [3] because a single number tells you localized vs extended instead of having to make a plot, but with python's capabilities not a big deal to make plots.

[5] Put in a defect spring: k --> k' on one bond, eg between masses j=1 and j=2. Matrix is now:

```
k+k'  -k'    0   0   [...]  0   -k
-k'   k+k'  -k   0   [...]  0    0
 0    -k    2k   0   [...]  0    0
 [...]
 0     0     0   0   [...] 2k   -k
-k     0     0   0   [...] -k   2k
```

Diagonalize it.

[6] Plot squares of components, or compute P_n. If k'>k you will find one localized mode. If you plot eigenvalues, will see a clump of closely spaced eigenvalues and a lonely eigenvalue higher than the rest. That's the localized mode. If k'<k I think there is no localized mode.

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More details:

[1] 1D chain of j=1,2,...N identical masses at positions x(j,t) connected by identical springs.

[2] Write down F=ma for each mass

```
m d^2 x(j,t)/dt^2  = -k [ x(j,t) - x(j+1,t) ] -k [ x(j,t) - x(j-1,t) ]
```

[3] Ansatz x(j,t) = v(j) e^(i w t) converts to algrbraic equations:

```
  m w^2 v(j  = 2k  v(j) - k v(j+1) -k v(j-1)
```

[4] This is just an eigenvalue problem: Tridiagonal matrix with "2k" along diagonal and "-k" above/below. m w^2 are eigenvalues. Use periodic boundary conditions. Matrix is:

```
     2k   -k   0   0   [...]  0   -k
     -k   2k  -k   0   [...]  0    0
      0   -k  2k   0   [...]  0    0
      [...]
      0    0   0   0   [...] 2k   -k
     -k    0   0   0   [...] -k   2k
```

[5] Call some routine (eg LAPACK) to diagonalize.

[6] Eigenvalues are actually known analytically

```
    m w^2 = 2k ( 1 - cos(q_n) )
```

where

```
    q_n = 2 pi n/N
    n = 1,2,3...N
```

Eigenvalues are doubly degenerate except n=N/2 and n=N.

[7] Eigenvectors are also known analytically

```
     v(q_n,j) = exp(i q_n j) / sqrt(N)
```

because of degeneracy, can make linear combinations so eigenvectors are real.

[8] Problem of a defect mass instead of a defect spring leads to a non-symmetric matrix. It is harder to find a diagonalizer for non-symmetric matrices.

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Physics:

[1] The eigenvectors/eigenvalues describe collective excitations of solid called 'phonons'

[2] Can do alternating springs k and k'. Will get two types of lattice vibrations: optical and acoustic phonons which differ according to how the energy (frequency) behaves as momentum q --->0.

[3] Problem is isomorphic to electron hopping on 1D chain of atoms. Matrix to be diagonalized is

```
      E   -t   0   0   [...]  0   -t
     -t    E  -t   0   [...]  0    0
      0   -t   E   0   [...]  0    0
      [...]
      0    0   0   0   [...]  E   -t
     -t    0   0   0   [...] -t    E
```

where E is atomic energy level and t is measure of overlap of wave functions on adjacent sites.

[4] Eigenvalue are "energy bands"

[5] If you alternate E ---> E1, E2 will get two bands separated by a band gap.

[6] If you write down matrix for 2d square lattice (put -t on any bond connecting adjacent sites in square array) and make histogram of eigenvalues you find that the number of eigenvalues at lambda=E diverges. This is called a 'van Hove singularity' and leads to instabilities like magnetism.

[7] If you write down matrix for 2d honeycomb lattice (put -t on any bond connecting adjacent sites in honeycomb array) you find Dirac fermions.

BOTTOM LINE OF [3]-[7]: many concepts, both basic and esoteric' of condensed matter physics come from a simple matrix diagonalization problem.