**Potential problem:**

The normalization constants $N_m$ can become very large (think of $E_0^m$)

**Solution:**

generate the normalized basis directly

- start with **$|\phi_0\rangle$** arbitrary, normalized, and then

$$|\phi_1\rangle = \frac{1}{N_1}\left(H|\phi_0\rangle - a_0|\phi_0\rangle\right).$$

$$|\phi_{m+1}\rangle = \frac{1}{N_{m+1}}\left(H|\phi_m\rangle - a_m|\phi_m\rangle - N_m|\phi_{m-1}\rangle\right) = \frac{|\gamma_{m+1}\rangle}{N_{m+1}}$$

The definition of $N_m$ is different, and no $b_m$:

$$\begin{aligned} a_m &= \langle\phi_m|H|\phi_m\rangle \\ N_m &= \langle\gamma_m|\gamma_m\rangle^{-1/2} \end{aligned}$$

Generate $|\gamma_m\rangle$ first, normalize to get $N_m$

The H-matrix is

$$\begin{aligned} \langle\phi_{m-1}|H|\phi_m\rangle &= N_m \\ \langle\phi_m|H|\phi_m\rangle &= a_m \\ \langle\phi_{m+1}|H|\phi_m\rangle &= N_{m+1} \end{aligned}$$

# Example in two dimensions: box with open boundaries

Constructing $H|f_n\rangle$ (open corresponds to hard walls)

State n stored in `f1[1:nx*ny]`
State $H|f_n\rangle$ in `f2[1:nx*ny]`

t = hopping (kinetic) matrix element
- consider hopping into all boxes j

labeling for 4*4 elements

| | | | |
|---|---|---|---|
| 13 | 14 | 15 | 16 |
| 9 | 10 | 11 | 12 |
| 5 | 6 | 7 | 8 |
| 1 | 2 | 3 | 4 |

```
function hoperation(f1,f2)
f2.=vpot.*f1
for j=1:nx*ny
   x=1+mod(j-1,nx)
   y=1+div(j-1,nx)
   if x!=1  f2[j-1]=f2[j-1]-t*f1[j]
   if x!=nx f2[j+1]=f2[j+1]-t*f1[j]
   if y!=1  f2[j-nx]=f2[j-nx]-t*f1[j]
   if y!=ny f2[j+nx]=f2[j+nx]-t*f1[j]
end
```

# One step in the iteration of the a and b coefficients

$$|\phi_1\rangle = \frac{1}{N_1}\big(H|\phi_0\rangle - a_0|\phi_0\rangle\big).$$

$$|\phi_{m+1}\rangle = \frac{1}{N_{m+1}}\big(H|\phi_m\rangle - a_m|\phi_m\rangle - N_m|\phi_{m-1}\rangle\big) = \frac{|\gamma_{m+1}\rangle}{N_{m+1}}$$

```
if m==1
   hoperation(f0,f1)
   aa[1]=dot(f0,f1)
   f1.=f1.-aa[1].*f0
   nn[2]=dot(f1,f1)^0.5
   f1.=f1./nn[2]
else
   hoperation(f1,f2)
   aa[m]=dot(f1,f2)
   f2.=f2.-aa[m].*f1-nn[m].*f0
   nn[m+1]=dot(f2,f2)^0.5
   f2.=f2./nn[m+1]
   f0.=f1
   f1.=f2
end
```

$$\begin{aligned} a_m &= \langle\phi_m|H|\phi_m\rangle \\ N_m &= \langle\gamma_m|\gamma_m\rangle^{-1/2} \end{aligned}$$

The method of constructing the normalized states directly

# The full basis and Hamiltonian construction

Random initial state

```
for i=1:n
   psi[i]=rand()-0.5
end
norm=1./(psi,psi)^0.5
Psi.=psi.*norm
```

Perform `niter` Lanczos steps and diagonalize

```
f0=copy(psi)
nn[1].=1.
for m=1:niter
   perform code on previous page
end
```

Diagonalize the matrix of size (niter+1)*(niter+1) made using
The diagonal and subdiagonal elements from aa and nn

# Calculation of the states

In order to calculate states (wave functions) we have to perform another Lanczos procedure, since we have not saved all the states $|f_n>$

If we want the m-th lowest state, we transform with the m-th eigenvector obtained in the diagonalization. The eigenvectors are in the matrix `states`; `vec=states(:,m)`

Normalized states $|\phi_n\rangle = {N_n}^{-1/2}|f_n\rangle$

```
f0.=psi
psi.=psi.*vec[1]
hoperation(f0,f1)
f1.=f1.-aa[0].*f0
psi.=psi.+vec[1].*f1./nn[2]^0.5
for i:2,niter-1
   hoperation(f1,f2)
   f2.=f2.-aa[i].*f1.-bb[i-1].*f0
   psi.=psi.+vec[i].*f2/nn[i+1]^0.5
   f0.=f1
   f1.=f2
end
```