PROBLEM SET 1 Due Friday April 12

Physics 140B– SPRING 2013

Analytic:

[1.] Suppose you have a system with eight sites, so the index labeling the fermion creation and destruction operators runs over eight possible values. Figure out the occupation number state which results from the following applications of the indicated operators. Choose as your convention that a given occupation number state is formed by acting on the vacuum state $|\text{vac}\rangle = |00000000\rangle$ with the lowest indices at the right of the string of creation operators. (The answers are almost obvious by 'intuition' except for the signs you get at the end. These you must be more careful with.)

$$\hat{c}_5^\dagger \hat{c}_4^\dagger \hat{c}_2^\dagger |\text{vac}\rangle = ?$$
$$\hat{c}_2^\dagger \hat{c}_4^\dagger \hat{c}_5^\dagger |\text{vac}\rangle = ?$$
$$\hat{c}_4^\dagger \hat{c}_5^\dagger |11000001\rangle = ?$$
$$\hat{c}_4^\dagger \hat{c}_5^\dagger |11001001\rangle = ?$$
$$\hat{c}_1^\dagger \hat{c}_2 |01001001\rangle = ?$$
$$\hat{c}_1^\dagger \hat{c}_4 |01001001\rangle = ?$$
$$\hat{c}_1^\dagger \hat{c}_5 |01001001\rangle = ?$$

[2.] In first quantized quantum mechanics it was often very useful to identify operators which commute with the Hamiltonian H. This helped in the search for eigenstates of H, since you knew they have to be eigenstates of the other operators as well. Consider the kinetic energy ('hopping') Hamiltonian from class (again for an eight site system as in problem #1):

$$H = -t \sum_{l=1}^{8} (c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1})$$

Does H commute with the number operator on site 3, $n_3 = c_3^\dagger c_3$? Does H commute with the *total* number operator $n_{\text{tot}} = \sum_{l=1}^{8} c_l^\dagger c_l$? Can you give an intuitive picture for your results?

[3.] Consider a six site system with the kinetic energy ('hopping') Hamiltonian from class (see problem #2). Write down all the states in the occupation number space with one electron. Show how H acts on each of these states. Write the matrix for H in this basis. What are its eigenvalues and eigenvectors?

[4.] Consider a six site system with the kinetic energy ('hopping') Hamiltonian from class (see problem #2). Write down all the states in the occupation number space with two electrons. Show how H acts on three of these states. (Pick any three you like.) Tough question with easy answer: What are the eigenvalues of the matrix for H in this two particle sector?! (You will get the answer numerically in problem #8 below).

[5.] Explain why, in problems #3,4 we can focus just on the individual subspaces of one or two electron states in diagonalizing H.

[**6.**] What are the eigenvalues of

$$H = -t\sum_{l=1}^{N}(c_{l+1}^{\dagger}c_l + c_l^{\dagger}c_{l+1}) + E\sum_{l=1}^{N}c_l^{\dagger}c_l$$

in the sector with one electron? This problem differs from #3, and what we did in class, only by the second ("E") term. Think about how this term affects the matrix for H. (Try acting with this H on a couple of the single particle states.)

[**7.**] Optional Compute the eigenvalues of

$$H = -t\sum_{l=1}^{N}(c_{l+1}^{\dagger}c_l + c_l^{\dagger}c_{l+1}) + E_1\sum_{l\ \text{odd}}c_l^{\dagger}c_l + E_2\sum_{l\ \text{even}}c_l^{\dagger}c_l$$

in the sector with one electron. This problem seems hard, perhaps, but it is actually the same mathematically as when we derived acoustic and optic phonons. There we found two phonon branches, and here you find the same thing, two electron energy bands centered at E_1 and E_2. Physically, this problem corresponds to figuring out the band structure of a material with two types of atoms with two different energy levels.

Numeric:

I will be available in room 106 Wednesday April 10, noon - 2 pm for questions about this assignment and, specifically, the numerical part.

[**8.**] Do problem numbers 3,4 numerically. That is, set up the matrices and call a numerical diagonalizer to get the eigenvalues and eigenvectors. One option is to use the diagonalization routines on the course website.

1//

Solns HW 6 P140A W2012

1 a) $c_5^\dagger c_4^\dagger c_2^\dagger |VAC\rangle = |01011000\rangle$

This has the order of our convention (lowest index on right)

b) $c_2^\dagger c_4^\dagger c_5^\dagger |VAC\rangle = -c_4^\dagger c_2^\dagger c_5^\dagger |VAC\rangle$

not in right order, need to adjust

$= +c_4^\dagger c_5^\dagger c_2^\dagger |VAC\rangle = -c_5^\dagger c_4^\dagger c_2^\dagger = -|01011000\rangle$

c) $c_4^\dagger c_5^\dagger |11000001\rangle = c_4^\dagger c_5^\dagger c_8^\dagger c_2^\dagger c_1^\dagger |VAC\rangle$

need to reorder so lowest on right

$c_4^\dagger c_5^\dagger c_8^\dagger c_2^\dagger c_1^\dagger = -c_5^\dagger c_4^\dagger c_8^\dagger c_2^\dagger c_1^\dagger = +c_5^\dagger c_8^\dagger c_4^\dagger c_2^\dagger c_1^\dagger$

$= -c_8^\dagger c_5^\dagger c_4^\dagger c_2^\dagger c_1^\dagger$

$\therefore \quad c_4^\dagger c_5^\dagger |11000001\rangle = -|11011001\rangle$

d) $c_4^\dagger c_5^\dagger |11001001\rangle = 0$

c_4 already occupied

e) $c_1^\dagger c_2 |01001001\rangle = c_1^\dagger c_2 c_8^\dagger c_5^\dagger c_2^\dagger |VAC\rangle$

$= -c_1^\dagger c_8^\dagger c_2 c_5^\dagger c_2^\dagger |VAC\rangle = +c_1^\dagger c_8^\dagger c_5^\dagger c_2 c_2^\dagger |VAC$

$= c_1^\dagger c_8^\dagger c_5^\dagger (1 - c_2^\dagger c_2) |VAC\rangle = -c_1^\dagger c_8^\dagger c_5^\dagger |VAC\rangle$

↑ gives ϕ on $|VAC\rangle$

$= +c_8^\dagger c_1^\dagger c_5^\dagger |VAC\rangle = -c_8^\dagger c_5^\dagger c_1^\dagger |VAC\rangle = -|10001001\rangle$

f) $c_1^\dagger c_4 |01001001\rangle = \phi$

↑ no fermion to destroy

g) $c_1^\dagger c_5 |01001001\rangle$

$= c_1^\dagger c_5 c_8^\dagger c_5^\dagger c_2^\dagger |VAC\rangle$

$= -c_1^\dagger c_8^\dagger c_5 c_5^\dagger c_2^\dagger |VAC\rangle = -c_1^\dagger c_8^\dagger c_2^\dagger |VAC\rangle$

$(1 - c_5^\dagger c_5)$

↑ ϕ

$= +c_8^\dagger c_1^\dagger c_2^\dagger |VAC\rangle$

$= -c_8^\dagger c_2^\dagger c_1^\dagger |VAC\rangle$

$= -|11000001\rangle$

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2 $c_1^\dagger c_2 c_3^\dagger c_3 = -c_1^\dagger c_3^\dagger c_2 c_3 = +c_3^\dagger c_1^\dagger c_2 c_3$

$= -c_3^\dagger c_1^\dagger c_3 c_2 = +c_3^\dagger c_3 c_1^\dagger c_2$

This shows $c_1^\dagger c_2$ commutes with $c_3^\dagger c_3 = n_3$

Pretty clearly the same argument works for other terms like $c_6^\dagger c_7$ etc. as long as c_3 is not involved. So let's look at

$$c_3^\dagger c_2 c_3^\dagger c_3 = -\underbrace{c_3^\dagger c_3^\dagger}_{0} c_2 c_3 = 0$$

$$c_3^\dagger c_3 c_3^\dagger c_2 = c_3^\dagger (1 - c_3^\dagger c_3) c_2$$

$$= c_3^\dagger c_2 - \phi = c_3^\dagger c_2$$

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so $[c_3^\dagger c_2, c_3^\dagger c_3] \neq 0 = -c_3^\dagger c_2$

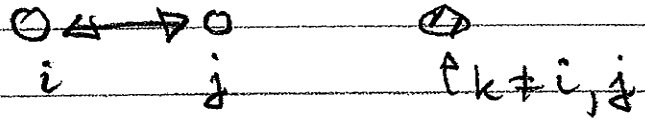
But notice this: $c_3^\dagger c_2 c_2^\dagger c_2 = c_3^\dagger (1 - c_2^\dagger c_2) c_2 = c_3^\dagger c_2$

and $c_2^\dagger c_2 c_3^\dagger c_2 = -c_2^\dagger c_3^\dagger c_2 c_2 = \phi$. Thus

$$[c_3^\dagger c_2, c_2^\dagger c_2] = +c_3^\dagger c_2$$

So $[c_3^\dagger c_2, c_2^\dagger c_2 + c_3^\dagger c_3] = 0$

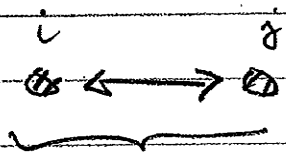
Summarizing: A hopping process between two sites i, j commutes with a number operator $\hat{n}_k$ not $\equiv$ on one of those sites:



A hopping process between two sites i, j

doesn't commute with n_i or n_j individually but does

commute with $n_i + n_j$ (intuitively reasonable)



$n_i + n_j$ conserved (but not n_i, n_j individually)

Together these facts imply $[\hat{H}, \hat{N}_{tot}] = \emptyset$

3. $H|100000\rangle = -t|010000\rangle - t|000001\rangle$

$H|010000\rangle = -t|100000\rangle - t|001000\rangle$

$H|001000\rangle = -t|010000\rangle - t|000100\rangle$

$H|000100\rangle$

$H|000010\rangle$ etc

$H|000001\rangle$

$$H = \begin{bmatrix} 0 & -t & 0 & 0 & 0 & -t \\ -t & 0 & -t & 0 & 0 & 0 \\ 0 & -t & 0 & -t & 0 & 0 \\ 0 & 0 & -t & 0 & -t & 0 \\ 0 & 0 & 0 & -t & 0 & -t \\ -t & 0 & 0 & 0 & -t & 0 \end{bmatrix}$$

As discussed in class eigenvalues $\epsilon_q = -2t\cos q$

$q = \frac{2\pi}{6}\{1,2,3,4,5,6\}$

Eigenvectors (general q) — specific $q = 2\pi$ — specific $q = \frac{2\pi}{6} = \frac{\pi}{3}$

$$\begin{bmatrix} 1 \\ e^{iq} \\ e^{2iq} \\ e^{3iq} \\ e^{4iq} \\ e^{5iq} \end{bmatrix} \quad \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad \begin{bmatrix} 1 \\ e^{i\pi/3} \\ e^{2i\pi/3} \\ e^{3i\pi/3} \\ e^{4i\pi/3} \\ e^{5i\pi/3} \end{bmatrix} \quad \ldots \text{ etc}$$

3//

4 $|110000\rangle$

$|101000\rangle$

$|100100\rangle$

$|100010\rangle$

$|100001\rangle$

only connect to two vectors if e^- adjacent ($1/2$ of hopping is "Pauli blocked")

$\hat{H}\,|011000\rangle = -t|101000\rangle - t|010100\rangle$

$|010100\rangle$

$\hat{H}\,|010010\rangle = \{-t|100010\rangle - t|001010\rangle$

$|010001\rangle \quad\quad -t|010100\rangle - t|010001\rangle$

$|001100\rangle$

$|001010\rangle$

$|001001\rangle$

$|000110\rangle$

$|000101\rangle$

$|000011\rangle$ = ·11

↑

15 states

There are 6 eigenstates of the $N=1$ sector of problem #3. One might expect the $N=2$ sector energies to be sums of those of $N=1$. But if $\epsilon_1, \epsilon_2, \epsilon_3, \ldots, \epsilon_6$ are the SIX eigenvalues in #3 this gives 36 two particle energies

$\epsilon_1+\epsilon_1 \quad \epsilon_1+\epsilon_2 \quad \epsilon_1+\epsilon_3 \quad \epsilon_1+\epsilon_4 \quad \epsilon_1+\epsilon_5 \quad \epsilon_1+\epsilon_6$

$\epsilon_2+\epsilon_1 \quad \epsilon_2+\epsilon_2 \quad \epsilon_2+\epsilon_3 \quad \epsilon_2+\epsilon_4 \quad \ldots$

$\epsilon_3+\epsilon_1 \quad \epsilon_3+\epsilon_2 \quad \epsilon_3+\epsilon_3$

$\vdots$

$\epsilon_6+\epsilon_1 \quad \epsilon_6+\epsilon_2$

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36 is too many! We have only 15 $N=2$ particle states! The key observations are that

1) $\epsilon_1 + \epsilon_2$ should not be counted separately from $\epsilon_2 + \epsilon_1$ because particles are indistinguishable

2) $\epsilon_1 + \epsilon_1$ is not allowed by Pauli.

This reduces the 36 to the correct 15

$$36 \longrightarrow 21 \longrightarrow 15$$

Indistinguishable Pauli

As discussed in Email, the subtlety is that actually the 15 $N=2$ eigenvalues are $\epsilon_1' + \epsilon_2'$, $\epsilon_1' + \epsilon_3'$ where the ϵ_i' are eigenvalues of

$$\begin{bmatrix} 0 & -t & 0 & 0 & 0 & +t \\ -t & 0 & -t & 0 & 0 & 0 \\ 0 & -t & 0 & -t & 0 & 0 \\ & & & \vdots & & \\ +t & 0 & 0 & 0 & -t & 0 \end{bmatrix}$$

APBC $N=1$ soln

8//

5 When $\hat{H}$ acts on an $N=1$ state it only connects to other $N=1$ states. Likewise for $N=2$, This is a consequence of $[\hat{H}, \hat{N}] = \emptyset$.

So $\hat{H}$ is block diagonal and its eigenstates/eigenenergy can be determined by looking at N sectors individually

$|n_1 n_2 n_3 n_4 n_5 n_6\rangle \leftarrow 2^6 = 64$ states (each $n_i = 0, 1$)

$|0\,0\,0\,0\,0\,0\rangle \leftarrow$ 1 state in $N=0$ sector

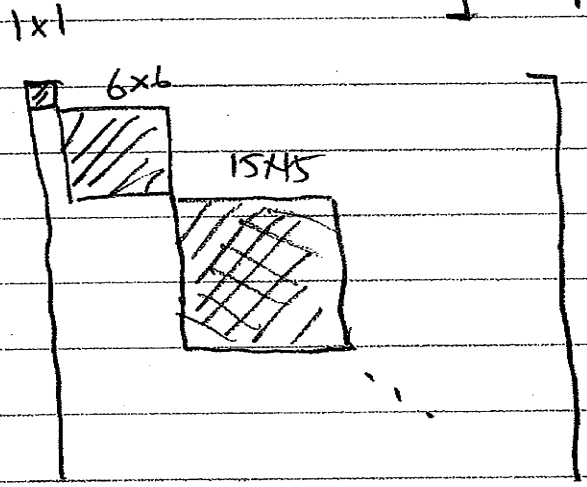
$|1\,0\,0\,0\,0\,0\rangle$
$|0\,1\,0\,0\,0\,0\rangle$
$|0\,0\,1\,0\,0\,0\rangle$
$\vdots$

$\leftarrow$ 6 states in $N=1$ sector

15 $N=2$ states
20 $N=3$ states
15 $N=4$ states
6 $N=5$ states
1 $N=6$ state

these sum to 64

$\hat{H} =$



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[6] The $E\sum_{1}^{N} c_\ell^\dagger c_\ell$ term adds an E to diagonal, eg

$$\hat{H}|100000\rangle = E|100000\rangle - t|010000\rangle - t|000001\rangle$$

So $\epsilon_q = E - 2t\cos q$

↑ if E added to diagonal of matrix
all eigenvalues shift by E
eigenvectors are unchanged.

[7] Matrix for H is pretty evidently

$$\hat{H} = \begin{bmatrix} E_1 & -t & 0 & 0 & 0 & \cdots \\ -t & E_2 & -t & 0 & 0 & \cdots \\ 0 & -t & E_1 & -t & 0 & \cdots \\ 0 & 0 & -t & E_2 & -t & \cdots \\ & & & & & \end{bmatrix}$$

The eigenvector problem $H|V\rangle = E|V\rangle$ is thus

$$E_1 V_\ell - t V_{\ell+1} - t V_{\ell-1} = \lambda V_\ell \qquad \ell \text{ odd}$$

$$E_2 V_\ell - t V_{\ell+1} - t V_{\ell-1} = \lambda V_\ell \qquad \ell \text{ even}$$

when written in component form

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Guess soln $V_\ell = Ae^{iq\ell}$ ℓ odd

$V_\ell = Be^{iq\ell}$ ℓ even

$E_1 A - tBe^{iq} - tBe^{-iq} = \lambda A$ ← $e^{iq\ell}$ terms cancelled out

$E_2 B - tAe^{iq} - tAe^{-iq} = \lambda B$

$$\begin{bmatrix} E_1 - \lambda & -2t\cos q \\ -2t\cos q & E_2 - \lambda \end{bmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

↑ determinant must vanish

$$\lambda^2 - (E_1 + E_2)\lambda + E_1 E_2 - 4t^2\cos^2 q = 0$$

$$\lambda = \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 16t^2\cos^2 q} \right]$$

The allowed q values go from $-\frac{\pi}{2}$ to $\frac{\pi}{2}$ instead of $-\pi$ to $+\pi$ and for each q there are 2 soln's $\pm\sqrt{\ }$ so we have the correct number of eigenvalues.

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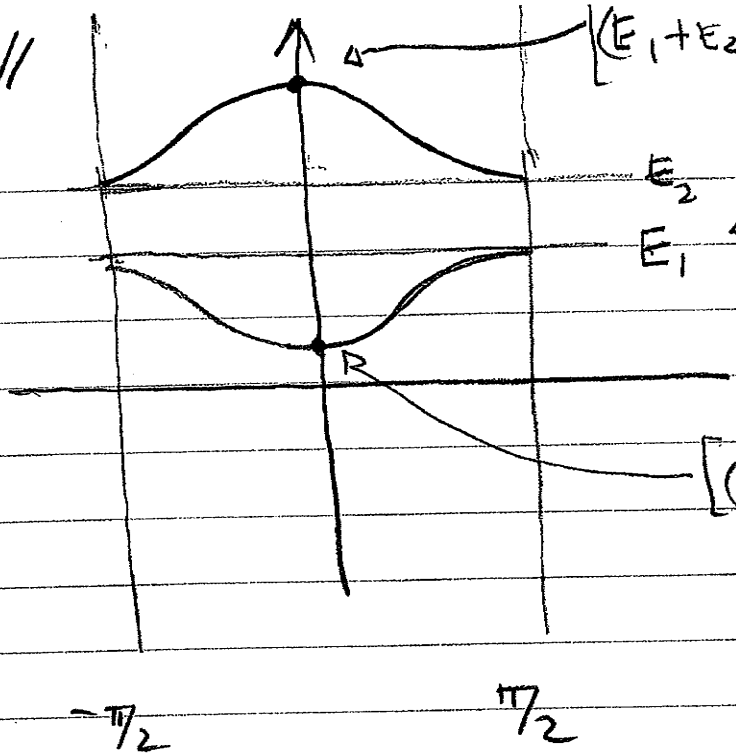


N = 8 case drawn

PROBLEM 8 - one electron on six sites code

```
/* oneelectronsixsites.c */

#include <stdio.h>
#include "nrutil.h"

void jacobi(float **a, int n, float d[], float **v, int *nrot);

int main() {

  int N  /* dimension of the matrix */
    , num_rot  /* number of Jacobi applied */
    , i, j;  /* temp. variables for counter */
  float ** A, ** eigenvectors, * eigenvalues;
  char format[] = "\n %7.3f";  /* format of output */
  float t;

  N=6;
  t=1.0;

  A = matrix( 1, N, 1, N);  /* must be a symmetric real matrix */
  eigenvectors = matrix( 1, N, 1, N);  /* eigenvectors as columns */
  eigenvalues = vector( 1, N);

 for( i = 1; i <= N; i++)
  for( j = 1; j <= N; j++)
   A[i][j]=0.0;

  for( i = 2; i <= N-1; i++){
   A[i][i-1]=-t;
   A[i][i+1]=-t;
   }
   A[1][N]=-t;
   A[1][2]=-t;
   A[N][N-1]=-t;
   A[N][1]=-t;

  jacobi( A, N, eigenvalues, eigenvectors, &num_rot);

  printf( "\nnumber of Jacobi applied: %i\neigenvalues:\n", num_rot);
  for( i = 1; i <= N; i++)
    printf(format, eigenvalues[i]);
  printf("\n");  /* next line */

  free_matrix( A, 1, N, 1, N);  free_matrix( eigenvectors, 1, N, 1, N);
  free_vector( eigenvalues, 1, N);

  return 0;
}
```

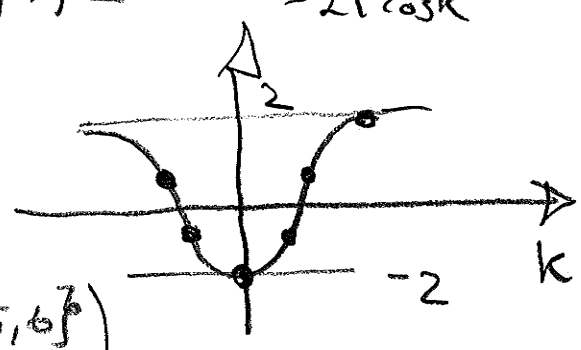
program gives eigenvalues

RESULTS → $-2, -1, -1, 1, 1, 2$

in agreement with $-2t\cos ka$

$k = \frac{2\pi}{6}\{-3,-1,0,1,2,3\}$

(equivalent to $k = \frac{2\pi}{6}\{1,2,3,4,5,6\}$)



Problem 8 : Getting $\hat{H}$ for 2 el. on 6 sites

STATE #	OCCUPATIONS	$\hat{H}$ connects to
1	$\|110000\rangle$	$-t\|2\rangle + t\|5\rangle$
2	$\|101000\rangle$	$-t\|1\rangle - t\|6\rangle + t\|9\rangle - t\|3\rangle$
3	$\|100100\rangle$	$-t\|7\rangle + t\|14\rangle - t\|2\rangle - t\|4\rangle$
4	$\|100010\rangle$	$-t\|8\rangle + t\|15\rangle - t\|5\rangle - t\|3\rangle$
5	$\|100001\rangle$	$-t\|9\rangle - t\|4\rangle$
6	$\|011000\rangle$	
7	$\|010100\rangle$	etc.
8	$\|010010\rangle$	
9	$\|010001\rangle$	
10	$\|001100\rangle$	
11	$\|001010\rangle$	
12	$\|001001\rangle$	
13	$\|000110\rangle$	
14	$\|000101\rangle$	
15	$\|000011\rangle$	

Problem 8 – the code

```
/* oneelectronsixsites.c */

#include <stdio.h>
#include "nrutil.h"

void jacobi(float **a, int n, float d[], float **v, int *nrot);

int main() {

  int N  /* dimension of the matrix */
    , num_rot  /* number of Jacobi applied */
    , i, j;  /* temp. variables for counter */
  float ** A, ** eigenvectors, * eigenvalues;
  char format[] = "\n %7.3f";  /* format of output */
  float t;

  N=15;
  t=1.0;

  A = matrix( 1, N, 1, N);  /* must be a symmetric real matrix */
  eigenvectors = matrix( 1, N, 1, N);  /* eigenvectors as columns */
  eigenvalues = vector( 1, N);

 for( i = 1; i <= N; i++)
  for( j = 1; j <= N; j++)
   A[i][j]=0.0;

A[1][2]   = -t;
A[1][9]   = +t;

A[2][1]   = -t;
A[2][6]   = -t;
A[2][3]   = -t;
A[2][12]  = +t;

A[3][7]   = -t;
A[3][14]  = +t;
A[3][2]   = -t;
A[3][4]   = -t;

A[4][8]   = -t;
A[4][15]  = +t;
A[4][5]   = -t;
A[4][3]   = -t;

A[5][9]   = -t;
A[5][4]   = -t;

A[6][2]   = -t;
A[6][7]   = -t;

A[7][3]   = -t;
A[7][6]   = -t;
A[7][10]  = -t;
A[7][8]   = -t;

A[8][4]   = -t;
A[8][11]  = -t;
A[8][7]   = -t;
A[8][9]   = -t;

A[9][5]   = -t;
A[9][12]  = -t;
```

```
A[9][8]   = -t;
A[9][1]   = +t;

A[10][7]  = -t;
A[10][11] = -t;

A[11][8]  = -t;
A[11][13] = -t;
A[11][10] = -t;
A[11][12] = -t;

A[12][9]  = -t;
A[12][14] = -t;
A[12][11] = -t;
A[12][2]  = +t;

A[13][11] = -t;
A[13][14] = -t;

A[14][12] = -t;
A[14][15] = -t;
A[14][13] = -t;
A[14][3]  = +t;

A[15][14] = -t;
A[15][4]  = +t;

 for( i = 1; i <= N; i++)
  for( j = 1; j <= N; j++)
  if (A[i][j]!=A[j][i]) printf(" symmetry violation %i %i ",i,j);

  jacobi( A, N, eigenvalues, eigenvectors, &num_rot);

  printf( "\nnumber of Jacobi applied: %i\neigenvalues:\n", num_rot);
  for( i = 1; i <= N; i++)
    printf(format, eigenvalues[i]);
  printf("\n");  /* next line */

  free_matrix( A, 1, N, 1, N);  free_matrix( eigenvectors, 1, N, 1, N);
  free_vector( eigenvalues, 1, N);

  return 0;
}
```

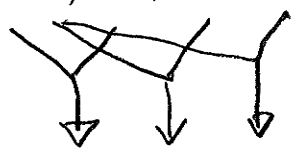
```
[rts@sherlock p140b]$ twoelectronsixsites.e
number of Jacobi applied: 667
eigenvalues:

   3.000
  -3.000
  -3.000
   3.000
  -2.000
  -1.000
   2.000
  -1.000
   0.000
  -0.000
   1.000
   1.000
   0.000
  -0.000
   0.000
```

Problem 8 — results

Note 2 electrons have energies generated by the 1 electron problem combined with Pauli principle and indistinguishability:

1 el levels $-2, -1, -1, 1, 1, 2$

2 el levels



$-3 \quad -3 \quad -1$

Ie take pairs of 1el levels $E_i + E_j$ with $i \neq j$ and i,j same as j,i

This correctly gives the 15 2 electron levels.