FYS3110 - Problem set 3

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a)

The matrix representation of $\hat{H}$ in the given basis follows from the formula

$$\hat{H} = -g \sum_{i=0}^{N-1} \Big(|i\rangle\langle i+1| + |i+1\rangle\langle i| \Big) - V|0\rangle\langle 0|$$

with the basis vectors inserted for $|i\rangle$ and $N = 4$. Each term in the sum contains two outer products of basis vectors that equals (keeping in mind that $|N\rangle \equiv |0\rangle$):

$$i = 0: \quad |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad |1\rangle\langle 0| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$i = 1: \quad |1\rangle\langle 2| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad |2\rangle\langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$i = 2: \quad |2\rangle\langle 3| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad |3\rangle\langle 2| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$i = 3: \quad |3\rangle\langle 0| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad |0\rangle\langle 3| = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

After adding all these matrices, the euqation for $\hat{H}$ yields

$$\hat{H} = -g \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} - V \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{H} = - \begin{pmatrix} V & g & 0 & g \\ g & 0 & g & 0 \\ 0 & g & 0 & g \\ g & 0 & g & 0 \end{pmatrix}$$

b)

The eigenvalues of the position operator $\hat{X}$ are the numbers labeling the atoms, hence

$$\hat{X}|i\rangle = i|i\rangle \quad for \quad i = 0, 1, 2, 3$$

These eigenvalues make up the diagonal of $\hat{X}$, while all the non-diagonal elements equal zero because the basis is orthogonal

$$\langle i|j\rangle = 0$$

The matrix-representation of $\hat{X}$ is thus

$$\hat{X} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

c)

I used Matlab to solve this problem for $N = 32$. The sum in the formula for the Hamiltonian $\hat{H}$ is computed in the same way as above with $g = 1$ and $V = 4$. The Matlab statement $[V, D] = eig(H)$ returns a diagonal matrix D with the eigenvalues of $\hat{H}$ and a matrix V whose columns are the corresponding eigenvectors. Since this is the Hamiltonian, the eigenvalues are the energies of the stationary states. The minimum element of D is therefore the lowest energy, i.e. the energy of the ground state. You can see from the output of my program that this is -4.4271. The energy-level diagram is plotted below.

d)

The probability of finding the electron on atom i is according to the Born rule

$$P(i) = |\langle i|\psi_g\rangle|^2$$

The inner product $\langle 0|\psi_g\rangle$ equals the first element of the column vector ψ_g, squaring this gives the probabilty of finding the electron on atom 0. The second element is the probability of finding it on atom 1. See program and output for results.

e)

I compute the expectation value in the script by constructing $\hat{X}$ and doing the calculation $\langle\psi_g|\hat{X}|\psi_g\rangle$. This gives the expectation value 1.6892, which is incorrect. The energies are symmetrically distributed around atom 0, so the expectation value should be zero. This incorrectness is caused by the fact that the script doesn't take into account that the atoms are on a ring, i.e. that atom N-1 is at the same distance from atom 0 as atom 1 etc.

Program and output

```
% parameters
g = 1;    % parameter associated with electron jumping
V = 4;    % potential atom 0
```

```
N = 32;  % number of atoms

% compute the Hamiltonian
H = zeros(N);
u = zeros(N,1);
v = zeros(N,1);
for i=1:N-1
    u(i) = 1;
    v(i+1) = 1;
    H = H + u*v' + v*u';
    u(i) = 0;
    v(i+1) = 0;
end

% last step (|N> = |0>)
u(N) = 1;
v(1) = 1;
H = H + u*v' + v*u';

% final form
H = -g*H - V*(v*v');

% compute eigenvectors and eigenvalues (energies)
[V,D] = eig(H);
energies = diag(D);

% plot energy-level diagram
levels = 0:N-1;
plot(levels, energies, 'bo')
xlabel('Level number')
ylabel('Energy')
title('Energy-level diagram')

% print lowest energy
lowest_energy = min(energies)

% ground state
ground_state = V(:,1);

% probabilites of finding electron on atom 0 and 1
prob0 = abs(ground_state(1))^2
prob1 = abs(ground_state(2))^2

% expectation value of position operator in ground state
X = diag(linspace(0,N-1,N));
exp_value = ground_state'*X*ground_state
```

Output

```
>> atoms_on_ring

lowest_energy =

   -4.4721

prob0 =

    0.8944

prob1 =

    0.0498

exp_value =

    1.6892
```

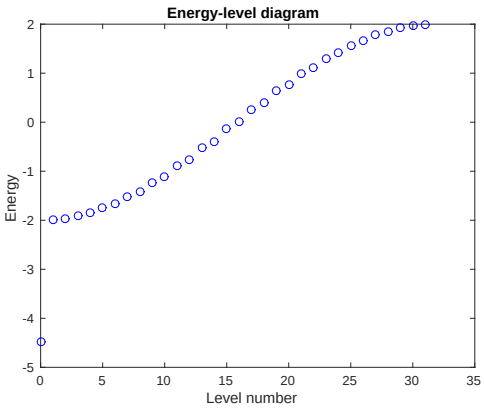

Figure 1: *Energy-level diagram*