Computational Physics
TU Dortmund - SuSe 2021

Solutions to exercise sheet 3

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0 Comprehension questions

The matrix A needs to be a square matrix and the number of columns needs to be the same as the number of elements in vector $\vec{v}$. Also the equation

$$A\vec{v} \neq 0 \tag{1}$$

needs to be true. The expression from the exercise sheet is the method of power iteration. Its proof is the reason why the expression converges to the eigenvector of A when increasing the power n.

1 Linear chain of elastic springs

1.1 Implementing a function that calculates all eigenfrequencies of a system

The system of N differential equations for the given problem is

$$\ddot{x}_1 = \frac{k_1}{m_1}(x_2 - x_1) \tag{2}$$

$$\ddot{x}_i = \frac{k_{i-1}}{m_i}(x_{i-1} - x_i) + \frac{k_i}{m_i}(x_{i+1} - x_i) \text{ for } i \in \{2, ..., N-1\} \tag{3}$$

$$\ddot{x}_N = \frac{k_{N-1}}{m_N}(x_{N-1} - x_N)\,. \tag{4}$$

From this we we can formulate the matrix A so that

$$\ddot{\vec{x}} = A\vec{x}\,. \tag{5}$$

- The first and last row of the matrix need to be set first, since there is no prior element for the first row and no following element for the last row
- The first row is set with "A.row(0).head(2) « -k(0) / m(0), k(0) / m(0)"
- The last row is set with "A.row(N - 1).tail(2) « k(N - 2) / m(N - 1), -k(N - 2) / m(N - 1)"
- The rest of the triagonal matrix A can be set with a for-loop

The eigenvalues λ_i of the matrix A are related to the eigenfrequencies $\omega_i \geq 0$ with

$$\lambda_i = -\omega_i^2\,. \tag{6}$$

1.2 Calculating the eigenfrequencies for a system with $N = 10$

The values for m_i, k_j and l_j are generated according to the rules on the exercise sheet. The matrix A is then generated by the priorly stated method from the m_i and k_j of the present system. The eigenfrequencies, calculated with eigen3, are presented in table 1.

Table 1: Eigenfrequencies of the present system

ω
3.95439
2.62228
1.95382
1.51083
1.17586
0.901365
0.663369
$1.23909 \cdot 10^{-8}$
0.44762
0.243446

2 Exercise 2: Lanczos algorithm

The Hamiltonian of the fermionic chain is given by

$$\mathcal{H} = -t \sum_{i=1}^{N} (|i\rangle\langle i+1| + |i+1\rangle\langle i|) + \epsilon |N/2\rangle\langle N/2| \tag{7}$$

2.1 Implementation of the Lanczos algorithm

The algorithm is implemented according to the lecture (script beckmann p.30).

2.2 Ground state and ground energy

For a chain of $N = 6$ lattice sites the Hamiltonian is given by

$$\mathcal{H} = \begin{pmatrix} 0 & -t & 0 & 0 & 0 & \boxed{\text{-t}} \\ -t & 0 & -t & 0 & 0 & 0 \\ 0 & -t & \epsilon & -t & 0 & 0 \\ 0 & 0 & -t & 0 & -t & 0 \\ 0 & 0 & 0 & -t & 0 & -t \\ \boxed{\text{-t}} & 0 & 0 & 0 & -t & 0 \end{pmatrix} \tag{8}$$

The entries marked in red represent the periodic boundary condition $|N+1\rangle = |N\rangle$. The ground state energy E_0 in dependence of the energy ϵ of the impurity is shown in Fig.1. For $\epsilon < 0$ the ground state energy tends towards ϵ, for $\epsilon > 0$ the impurity has no impact on the ground state energy.
The particle density for $\epsilon = -20, 2, 20$ is shown in Fig.2. For very small values the particles are located at the impurity, for large values the impurity has a repulsive character, so no particles are located there. For $\epsilon = 0$ the particles are uniformly distributed.

2.3 Organization of storage

Since $\mathcal{H}$ only contains a small number of non-zero elements, a sparse-matrix could be used.

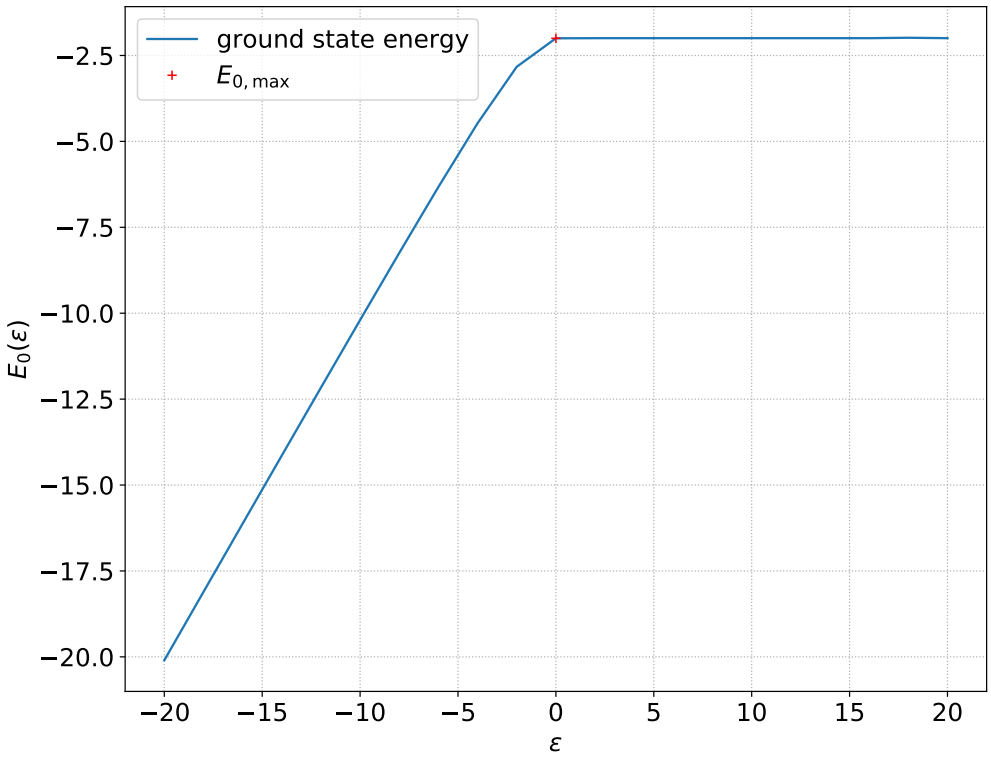

Figure 1: Ground state energy for different ϵ's.

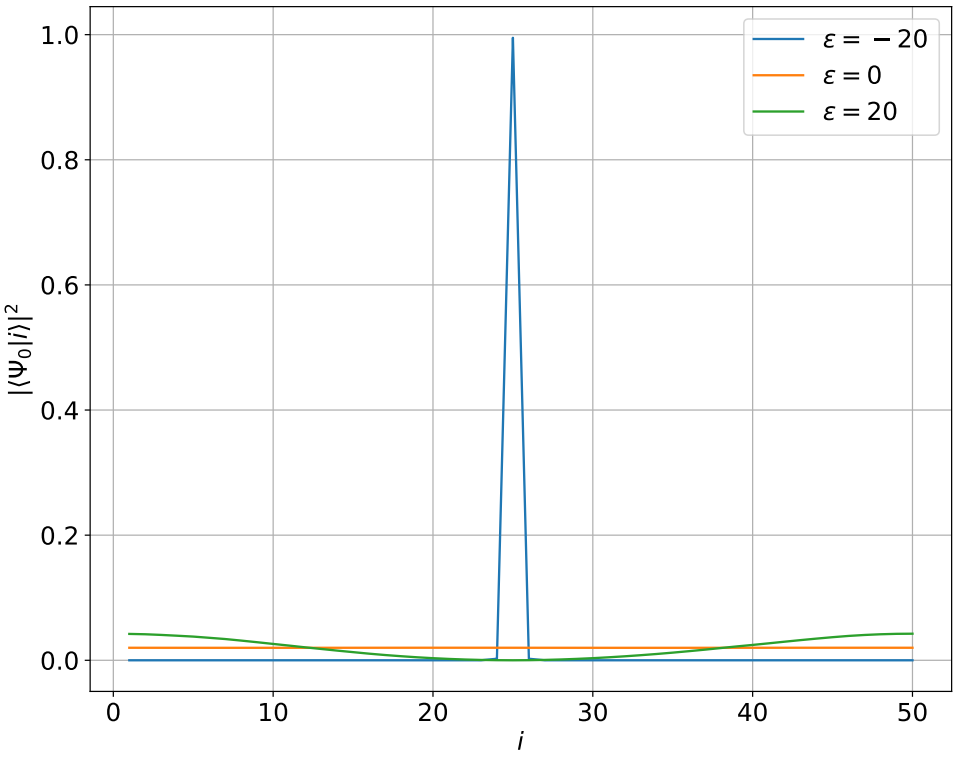

Figure 2: Particle density for $\epsilon = -20, 0, 20$.