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Exercise Sheet No. 3
"Computational Condensed Matter Theory"

7 Tight-binding chain (1d) with disorder

Consider the tight-binding Hamiltonian

$$\hat{H} = -\sum_{\langle k,l\rangle} t_{kl} c_k^\dagger c_l + \sum_{l\in\mathcal{L}} \epsilon_l c_l^\dagger c_l \tag{1}$$

$c_l^\dagger, c_l$ denote fermionic creation and annihilation operators acting on site l of a 1d chain with $L = 500$ sites. The hopping matrix t_{kl} connects nearest neighbors, only. Assume periodic boundary conditions.

a) On-site disorder

First consider a uniform hopping $t_{kl} = t$ and random "on-site energies" ϵ_l. The values for ϵ_l are uniformly normal random numbers with zero mean and a standard deviation $\sigma = 0.5t$.
Calculate, by exact diagonalization, the spectrum and the corresponding density of states (DOS) for three different disorder realizations. Visualize several eigenfunctions. Discuss your observations and the physical implications.
Calculate the DOS averaged over an ensemble of 1000 disorder realizations.

b) Off-diagonal disorder

Now consider pure off-diagonal disorder $\epsilon_l = 0$ and $t_{l,l+1} = t + \delta t_l$ at random values for δt_l chosen to be uniformly distributed from an interval $[-\frac{W}{2}, \frac{W}{2}]$. As disorder strength choose $W = t$
Again, average the DOS over 1000 disorder configurations. Compare your results with the previous on-site disorder case. Is the type of disorder distribution of importance?

Useful Matlab function: `normrnd`, `rand`.

8 Arnoldi method

In preparation for upcoming problems we implement and study methods to construct an orthonormal basis of the Krylov subspace $\mathcal{K}_m(\mathbf{v})$,

$$\mathcal{K}_m(\mathbf{v}) = \mathrm{span}\left\{\mathbf{v}; A\mathbf{v}; \ldots; A^{m-1}\mathbf{v}\right\}.$$

a) Classical Gram-Schmidt Orthogonalization

Write a function which takes as arguments a set of vectors and performs a classical Gram-Schmidt orthogonalization (Alg. 1) of these vectors.
Now consider a Hamiltonian as described in exercise **7a)**. Using the starting vector $\mathbf{v} = (1, 0, 1, 0, \ldots 0)^{\mathrm{T}}$, construct a basis $\left\{\mathbf{v}; \hat{H}\mathbf{v}; \ldots; \hat{H}^{m-1}\mathbf{v}\right\}$ for $m = 25$ explicitly. Use the Gram-Schmidt method to explicitly calculate an orthonormal basis set $\{\mathbf{v}_i\}$. Calculate the matrix elements $H^{\mathrm{a}}_{ij} = \mathbf{v}_i^{\mathrm{T}} \hat{H} \mathbf{v}_j$ and diagonalize the matrix H^{a}.

8 Arnoldi method (continued)

b) Modified Gram-Schmidt Orthogonalization

Write a function analogous to the previous exercise that implements the modified Gram-Schmidt orthogonalization (Alg. 2). Use this new function to calculate a new orthonormal basis $\{\mathbf{v}_i\}$, the corresponding matrix elements H^{b}_{ij} and the eigenvalues of H^{b}. Use the same initial basis $\left\{\mathbf{v}; \hat{H}\mathbf{v}; \ldots; \hat{H}^{m-1}\mathbf{v}\right\}$ as in **a)**.

c) Arnoldi Method

Now implement the Arnoldi method to obtain a third basis: Write a function which takes as arguments a matrix A, an initial vector $\mathbf{v}_1 = \mathbf{v}/||\mathbf{v}||$, and the size of the Krylov subspace m. Using the algorithm introduced in the lecture the function should return the upper Hessenberg matrix $\bar{H}$ and the matrix $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]$.
Using this function, calculate V_m and $\bar{H}$ for the Hamiltonian of exercise **7a)**, $\mathbf{v} = (1, 0, 1, 0, \ldots 0)^{\mathrm{T}}$ and $m = 25$. Calculate the spectrum of the matrix H^{c}, which is obtained from $\bar{H}$ by eliminating the last row.

d) Comparison of Methods

Test the orthogonality of the vectors $\{\mathbf{v}_i\}$ for all three given methods and compare. For the Arnoldi method, examine the off-tridiagonal elements of the matrix H^{c}. Compare the spectra of H^{a}, H^{b}, and H^{c} to the spectrum of the full Hamiltonian $\hat{H}$. Discuss your results. Why do people prefer modified Gram-Schmidt over classical Gram-Schmidt for orthonormalization? Why do people prefer the Arnoldi method of exercise **c)** to the explicit construction of the Krylov space done in exercises **a)** and **b)**?

9* Lanczos Method

The Lanczos method for symmetric matrices as introduced in the lecture, enables the calculation of selected eigenvalues of huge systems not treatable by full diagonalization. Consider the Hamiltonian for a 1d chain with on-site disorder from exercise **7a)**, but construct it as a sparse matrix for a system size $L = 100\,000$. Implement and apply the Lanczos method to calculate the lowest lying eigenvalue and eigenvector for both H and H^2. Terminate if the eigenvalue differs by less than 10^{-5} (absolute value) between two iterations. Visualize the eigenvectors. Can one trust these results?

Algorithm 1:
Classical Gram-Schmidt Orthogonalization

1. **Input:** Set of vectors $\mathbf{u}_i$, $i \in \{1, \ldots, m\}$
2. **Output:** $V_m = [\mathbf{v}_1, \ldots, \mathbf{v}_m]$
3. $\mathbf{v}_1 \leftarrow \mathbf{u}_1/||\mathbf{u}_1||$
4. For $j = 2, \ldots, m$ Do
   (a) $\mathbf{w} \leftarrow \mathbf{u}_j$
   (b) For $k = 1, \ldots, j-1$ Do
      i. $\mathbf{w} \leftarrow \mathbf{w} - (\mathbf{v}_k^{\dagger}\mathbf{u}_j)\mathbf{v}_k$
   (c) End-For
   (d) $\mathbf{v}_j \leftarrow \mathbf{w}/||\mathbf{w}||$
5. End-For

Algorithm 2:
Modified Gram-Schmidt Orthogonalization

1. **Input:** Set of vectors $\mathbf{u}_i$, $i \in \{1, \ldots, m\}$
2. **Output:** $V_m = [\mathbf{v}_1, \ldots, \mathbf{v}_m]$
3. $\mathbf{v}_1 \leftarrow \mathbf{u}_1/||\mathbf{u}_1||$
4. For $j = 2, \ldots, m$ Do
   (a) $\mathbf{w} \leftarrow \mathbf{u}_j$
   (b) For $k = 1, \ldots, j-1$ Do
      i. $\mathbf{w} \leftarrow \mathbf{w} - (\mathbf{v}_k^{\dagger}\mathbf{w})\mathbf{v}_k$
   (c) End-For
   (d) $\mathbf{v}_j \leftarrow \mathbf{w}/||\mathbf{w}||$
5. End-For