

Exercise Sheet No. 4

“Computational Condensed Matter Theory”

10 Wave packet dynamics

Consider the tight-binding Hamiltonian

$$\hat{H} = - \sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l$$

with periodic boundary conditions; \(c_k^\dagger, c_k\) denote fermionic creation and annihilation operators acting on site \(k\) of a one-dimensional chain. The hopping matrix \(t_{kl}\) connects nearest neighbors, only. In the following we consider uniform hopping \(t_{kl} = \tilde{t}\).

a) Clean system, full matrix exponential

For a time independent Hamiltonian \(\hat{H}\) the wave function \(\psi\) at time \(t\) is given by

$$\psi(t) = e^{-i\hat{H}t} \psi(0).$$

Examine the time evolution of a Gaussian wave packet centered at \(x_0\)

$$\psi(0) = \exp \left( - \frac{(x - x_0)^2}{2\sigma^2} \right) \exp(ik_0x)$$

moving along the 1d chain.

For a small system size of \(L = 100\) sites, consider \(k_0 = \frac{\pi}{2}\), \(\sigma = 10\) and \(x_0\) in the middle of the chain. Choose the lattice constant \(a\) as unit of length, \(\tilde{t}\) as unit of the energy and \(1/\tilde{t}\) as unit of time. Using the function \(\expm()\) of Matlab, which implements a matrix exponential, calculate the wave function for times \(t = 0 \ldots 50\) with time steps \(\Delta t = 0.5\).

Generate an animation showing the evolution of \(|\psi(x,t)|^2\) with time.

b) Clean system, Krylov space method

For huge matrices the calculation of the matrix exponential will be computational demanding or impossible. A way to overcome this problem is to resort to iterative methods:

1. Use the Arnoldi method to construct an orthonormal basis of the Krylov subspace \(\mathcal{K}_m(v_1) = \text{span} \{ v_1; Av_1; \ldots; A^{m-1}v_1 \} \) for the Hamiltonian and the wave function \(\psi_{t_0} = \psi(0)\) as starting vector \(v_1\).

2. Calculate the matrix \(H\) obtained from the Hessenberg matrix \(\tilde{H}\) by deleting its last row, and the matrix \(V_m = [v_1, v_2, \ldots, v_{m-1}]\).

3. Calculate the time evolution for a time step \(\Delta t\) in the Krylov subspace, \(y = e^{-iH\Delta t}e_1\), \(e_1 = (1, 0, 0, 0, \ldots, 0)^T\), where \(e_1 \in \mathcal{K}_m(v_1)\). Note that \(V_m e_1 = v_1\).

4. Using \(V_m\) and \(y\), calculate the new wave function \(\psi_{t+1} = \psi(t_i + \Delta t)\).

5. Repeat at step 1. with \(\psi_{t_{i+1}}\) as new starting vector \(v_1\).

\(^1\)Here \(H\) denotes the upper triangular matrix, not to be confused with the orginal Hamiltonian \(\hat{H}\)!
By repeatedly applying the steps above calculate the time evolution of $|\psi(x,t)|^2$ as in exercise 10a) for the same parameters and a Krylov subspace of $m = 10$. Compare the two methods by an animation showing the results of both methods in one graph. Examine and discuss the scaling of both methods with growing system size $L$.

c) Examine the Krylov space method a little closer, by using the algorithm but now without rebuilding the Krylov subspace and replacing $\Delta t$ in the exponential of step 3 accordingly. Compare the evolution of $|\psi(x,t)|^2$ with exercise 10b). Inspect $y$ as soon as the two methods deviate.

d) Consider again the full algorithm of exercise 10b). Instead of using a fixed $m$, dynamically adjust $m$ in each iteration step, so that

$$|y_m| + |y_{m-1}| < \text{tolerance} \quad (y_m \text{ denotes the } m\text{-th element of } y). \quad (3)$$

(Note the plus sign!) Investigate the behavior of this modified algorithm for different time steps of $\Delta t = 0.5, 5, 10$. Increase the system size $L$ and $t_{\text{max}}$ accordingly.

11 Wave packet dynamics in the presence of disorder

Consider the tight-binding Hamiltonian including on-site disorder

$$\hat{H} = -\sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l + \sum_{l \in L} \delta \varepsilon_l c_l^\dagger c_l$$

with periodic boundary conditions. Consider a uniform hopping $t_{kl} = \bar{t}$ and random “on-site energies” $\delta \varepsilon_l$. The values for $\delta \varepsilon_l$ are uniformly distributed random values from an interval $[-\frac{W}{2}, \frac{W}{2}]$. For a 1d-system of $L \geq 1000$ sites use the Krylov space method to examine the time evolution of $|\psi(x,t)|^2$ for a weak disorder strength $W = 0.1\bar{t}$ and strong disorder $W = 2\bar{t}$. Compare, interpret and discuss the results.

12* Simulation of a quantum interference experiment

Assume a clean 2d square lattice described by a tight-binding Hamiltonian with a hopping matrix connecting nearest neighbors only.

Simulate a double-slit experiment in this system:

- Consider how to model a double-slit geometry by modifying the hopping matrix elements.
- Choose a suitable starting vector for your time evolution.
- Calculate the time evolution $\psi(\mathbf{r},t)$ using the Krylov method of exercise 10b).
- Visualize the wave function intensity $|\psi(\mathbf{r},t)|^2$ over time.
- Select an appropriate time $t$ to best observe the interference pattern.

Hint: Beware of boundary effects.

Wir wünschen allen frohe Feiertage und einen guten Rutsch ins neue Jahr!