

## Exercise Sheet No. 4 “Computational Condensed Matter Theory”

### 10 Wave packet dynamics

Consider the tight-binding Hamiltonian

$$\hat{H} = - \sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l \quad (1)$$

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  $x_0$

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

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  $t = 0 \dots 50$  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  $\mathcal{K}_m(\mathbf{v}_1) = \text{span}\{\mathbf{v}_1; A\mathbf{v}_1; \dots; A^{m-1}\mathbf{v}_1\}$  for the Hamiltonian and the wave function  $\psi_{t_0} = \psi(0)$  as starting vector  $\mathbf{v}_1$ .
2. Calculate the matrix  $H$  obtained from the Hessenberg matrix  $\bar{H}$  by deleting its last row, and the matrix  $V_m = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{m-1}]$ .
3. Calculate the time evolution for a time step  $\Delta t$  in the Krylov subspace<sup>1</sup>,  $\mathbf{y} = e^{-iH\Delta t} \mathbf{e}_1$ ,  $\mathbf{e}_1 = (1, 0, 0, \dots, 0)^T$ , where  $\mathbf{e}_1 \in \mathcal{K}_m(\mathbf{v}_1)$ . Note that  $V_m \mathbf{e}_1 = \mathbf{v}_1$ .
4. Using  $V_m$  and  $\mathbf{y}$ , calculate the new wave function  $\psi_{t_{i+1}} = \psi(t_i + \Delta t)$ .
5. Repeat at step 1. with  $\psi_{t_{i+1}}$  as new starting vector  $\mathbf{v}_1$ .

<sup>1</sup>Here  $H$  denotes the upper triangular matrix, not to be confused with the original 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  $\mathbf{y}$  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

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

(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  $t_{max}$  accordingly.

### 11 Wave packet dynamics in the presence of disorder

Consider the tight-binding Hamiltonian including on-site disorder

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

with periodic boundary conditions. Consider a uniform hopping  $t_{kl} = \tilde{t}$  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  $W = 0.1\tilde{t}$  and strong disorder  $W = 2\tilde{t}$ . 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!

