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Exercise Sheet No. 4
"Computational Condensed Matter Theory"

10 **Wave packet dynamics**

Consider the tight-binding Hamiltonian

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

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 independendent Hamiltonian $\hat{H}$ the wave function ψ 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

$$\psi(0) = \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)\exp(ik_0 x) \tag{2}$$

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 $t = 0 \ldots 50$ 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 $\mathcal{K}_m(\mathbf{v}_1) = \text{span}\left\{\mathbf{v}_1; A\mathbf{v}_1; \ldots; A^{m-1}\mathbf{v}_1\right\}$ 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 $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_{m-1}]$.

3. Calculate the time evolution for a time step Δt in the Krylov subspace[1] , $\mathbf{y} = e^{-iH\Delta t}\mathbf{e}_1$, $\mathbf{e}_1 = (1, 0, 0, \ldots, 0)^T$, 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 $\mathbf{v}_1$.

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[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 Δt 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

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

(Note the plus sign!) Investigate the behavior of this modified algorithm for different time steps of $\Delta t = 0.5, 5, 10$. Adjust 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!