19.2.4 Time Evolution of Quantum Systems

Dynamical correlation functions are an important aspect in the description of interacting quantum systems and, in many cases, are directly related to experimental results, in particular spectroscopy data. On the other hand, new experimental setups and techniques led to an increased interest in the real time dynamics of quantum systems. Chebyshev expansion is applicable also in this situation.

Starting from the time dependent Schrödinger equation,

$$\mathrm{i}\partial_t|\psi\rangle = H|\psi\rangle \;, \tag{19.71}$$

the approach is surprisingly simple: Assuming that at time $t = 0$ the system is in the state $|\psi_0\rangle$, its state at a later time is

$$|\psi_t\rangle = \mathrm{e}^{-\mathrm{i}Ht}|\psi_0\rangle \;, \tag{19.72}$$

and the problem translates into calculating the time evolution operator $U(t) = \exp(-\mathrm{i}Ht)$ for a given Hamiltonian H and time t. Using the rescaling introduced in (19.7), we can expand $U(t)$ in a series of Chebyshev polynomials [39, 40, 41],

$$U(t) = \mathrm{e}^{-\mathrm{i}(a\widetilde{H}+b)t} = \mathrm{e}^{-\mathrm{i}bt}\left(c_0 + 2\sum_{k=1}^{N} c_k T_k(\widetilde{H})\right) \;, \tag{19.73}$$

where the expansion coefficients c_k are given by

$$c_k = \int_{-1}^{1} \frac{T_k(x)\mathrm{e}^{-\mathrm{i}axt}}{\pi\sqrt{1-x^2}}\,\mathrm{d}x = (-\mathrm{i})^k J_k(at) \;, \tag{19.74}$$

and $J_k(at)$ denotes the Bessel function of order k. The Chebyshev polynomials of the Hamiltonian, $T_k(\widetilde{H})$, are calculated with the recursion we introduced earlier, see (19.3). Thus, the wave function at a later time is obtained simply through a set of MVMs with the Hamiltonian.

Asymptotically the Bessel function behaves as

$$J_k(z) \sim \frac{1}{k!}\left(\frac{z}{2}\right)^k \sim \frac{1}{\sqrt{2\pi k}}\left(\frac{\mathrm{e}z}{2k}\right)^k \tag{19.75}$$

for $k \to \infty$, hence for $k \gg at$ the expansion coefficients c_k decay superexponentially and the series can be truncated with negligible error. With an expansion order of $N \gtrsim 1.5at$ we are usually on the safe side. Moreover, we can check the quality of our approximation by comparing the norms of $|\psi_t\rangle$ and $|\psi_0\rangle$. For sparse matrices the whole time evolution scheme is therefore linear in both, the matrix dimension and the time.

The Chebyshev expansion method converges much faster than other time integration methods, in particular, it is faster than the popular Crank-Nicolson method

[42]. Within this approach the time interval t is divided into small steps $\Delta t = t/N$, and the wave function is propagated in a mixed explicit/implicit manner,

$$(1 + \tfrac{1}{2}\mathrm{i}H\Delta t)|\psi_{n+1}\rangle = (1 - \tfrac{1}{2}\mathrm{i}H\Delta t)|\psi_n\rangle \; . \tag{19.76}$$

Thus, each step requires both a sparse MVM and the solution of a sparse linear system. Obviously, this is more complicated than the Chebyshev recursion, which requires only MVMs. In the Crank-Nicolson method the time evolution operator is approximated as

$$U(t) = \left(\frac{1 - \mathrm{i}Ht/(2N)}{1 + \mathrm{i}Ht/(2N)}\right)^N \; . \tag{19.77}$$

In Fig. 19.6 we compare this approximation with the Chebyshev approximation by replacing H with the real variable x (this is equivalent to working with a diagonal matrix H). In both cases we consider time $t = 10$ and expansion order $N = 15$. Whereas the Chebyshev result agrees perfectly with the exact result $\exp(\mathrm{i}xt)$, the Crank-Nicolson approximation needs much higher N to achieve the same accuracy ($N \approx 90$).

Having explained the time evolution algorithm, let us now consider a specific example: the formation of a polaron on an one-dimensional lattice. The Hamiltonian for this problem was introduced at the beginning of this chapter, see (18.3). The polaron problem corresponds to the case of a single electron interacting with finite frequency lattice vibrations, i.e., we can omit the spin indices and the Hubbard term does not contribute. Bonča, Trugman and co-workers [43, 44] introduced a highly efficient variational basis for the polaron problem, which can be used to study its ground-state properties and lowest excitations on an infinite lattice, as well as the

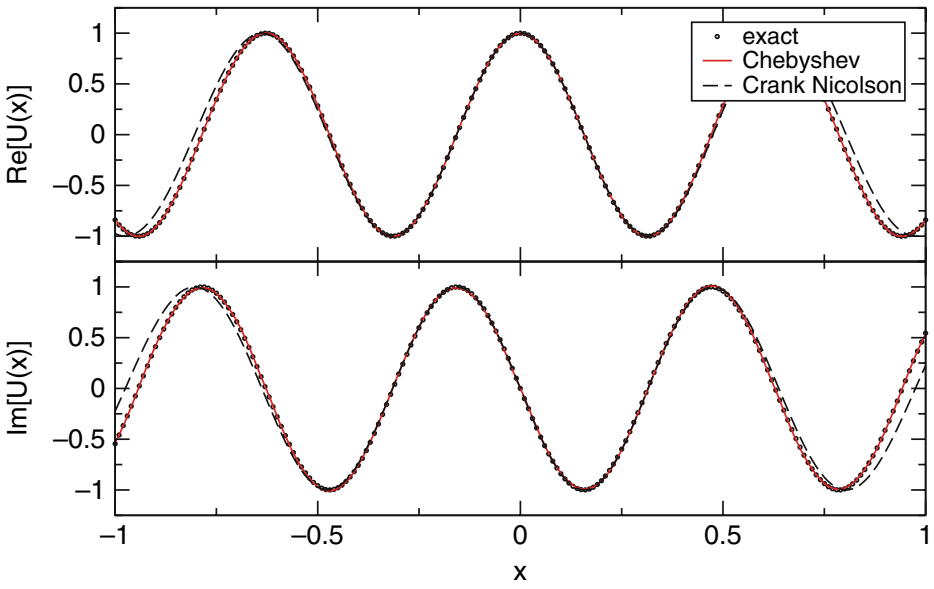

Fig. 19.6. Comparison of the Chebyshev and the Crank-Nicolson approximation of the function $U(t) = \exp(\mathrm{i}xt)$ with $t = 10$ and expansion order $N = 15$

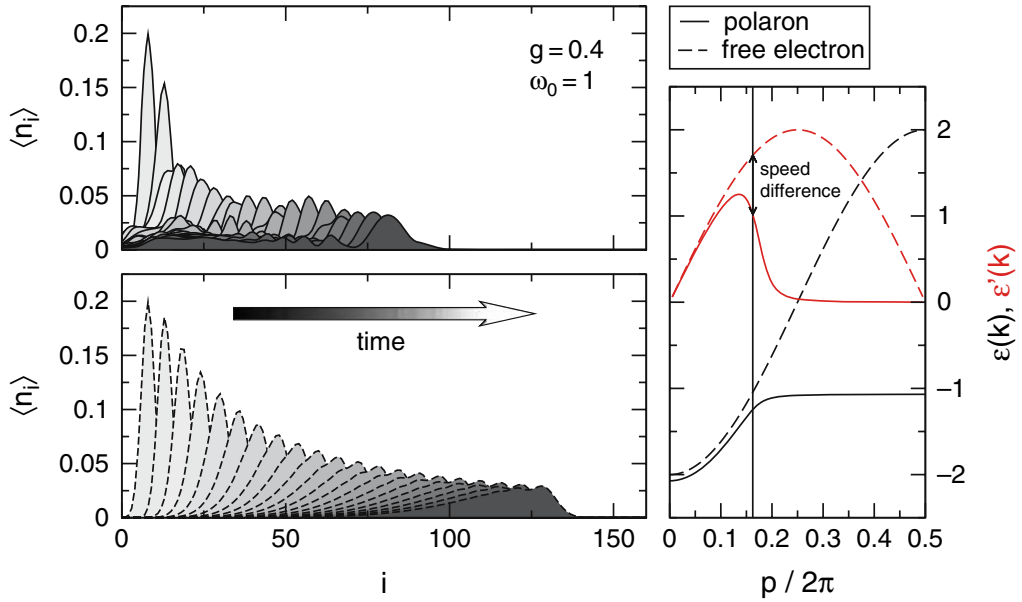

Fig. 19.7. Formation of a polaron for electron-lattice coupling $g = 0.4$ and phonon frequency $\omega_0 = 1$ (**upper panel**), compared to the motion of a non-interacting wave packet (**lower panel**). The right panel shows the underlying dispersions (*lower curves*) and velocities (*upper curves*)

quantum dynamics of such a system (for a recent review see also [45]). In Fig. 19.7 we show the time evolution of a single-electron wave packet

$$|\psi_0\rangle = \sum_j \mathrm{e}^{\mathrm{i}pj-(j-j_0)^2/(2\sigma^2)}\, c_j^\dagger|0\rangle\ , \tag{19.78}$$

where in the upper and lower panels the electron-phonon coupling g is finite or zero, respectively. For finite g, within the first few time steps a polaron is formed, which then travels at lower speed, compared to the non-interacting wave packet. The speed difference is given by the difference of the derivatives $\varepsilon'(k)$ of the underlying dispersions $\varepsilon(k)$ at the mean momentum p, see right hand panel. The Chebyshev expansion method allows for a fast and reliable simulation of this interesting problem.

19.3 KPM in Relation to other Numerical Approaches

19.3.1 KPM and CPT

The spectrum of a finite system of L sites, which we obtain through KPM, differs in many respects from that of an infinite system, $L \to \infty$, especially since for a finite system the lattice momenta $K = \pi\, m/L$ and the energy levels are discrete. While we cannot easily increase L without reaching computationally inaccessible Hilbert space dimensions, we can try to extrapolate from a finite to the infinite system.

With the Cluster Perturbation Theory (CPT) [46, 47, 48] a straightforward way to perform this task approximatively has recently been devised. In this scheme one