Density Matrix Theory

Prof. Andrea Donarini 5.0.21, Tuesdays, 10:15

Sheet 3

1. Spectral analysis of the density matrix dynamics (analytics)

Let us consider a quantum ring described by the Hamiltonian:

$$H = \sum_{\alpha=1}^{N} \left[\varepsilon c_\alpha^\dagger c_\alpha + b(c_{\alpha+1}^\dagger c_\alpha + c_\alpha^\dagger c_{\alpha+1}) \right]$$

where $c_\alpha^\dagger$ creates a (spinless) electron on the α site and we impose periodic boundary conditions: $c_{\alpha+N} = c_\alpha$.

1. Give the analytical form of the time evolution of the density matrix in the position representation as a function of a generic initial condition $\rho^0_{\alpha\beta}$ also given in the position representation.

2. Calculate analytically the Fourier transform of the previous result:

$$\tilde{\rho}_{\alpha\beta}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}t \, \rho_{\alpha\beta}(t) \, \mathrm{e}^{i\omega t}$$

   and prove that it is a sum of delta functions centered at the Bohr frequencies of the system.

3. The populations always have a zero frequency component, why?

4. Consider now different initial conditions: i) the localized pure state $|\alpha\rangle\langle\alpha|$; ii) the pure state $|\psi\rangle\langle\psi|$ with $|\psi\rangle = a|\ell_1\rangle + b|\ell_2\rangle$, where $|\ell_i\rangle$ is the complex eigenvector of H introduced in the previous exercise Sheet. What are the spectral components in the evolution of the density matrix in these two cases?

5. The dynamics of the case ii) of the previous point can be described as a rotation in space and the system periodically returns to its initial condition (see previous Sheet). Prove that this is also true for the localized initial condition i) of the previous point only for specific number of sites. In particular, the system returns to the localized state $|\alpha\rangle\langle\alpha|$ after a finite time for $N = 2, 3, 4, 6$ but not for $N = 5$.

   Hint: Construct explicitly the spectrum of the system and the Bohr frequencies. Then analyze the ratio of the Bohr frequencies...

Please, turn the page!

2. Spectral analysis of the density matrix dynamics (numerics)

Consider now the numerical solution for the evolution of the density matrix presented in the previous exercise. Even if we know the evolution exactly, we can calculate it only for a finite and discrete set of times $[0, \delta t, 2\delta t, \dots, (N-1)\delta t]$. This fact sets some limitation over the numerical spectral analysis of the dynamics of the density matrix.

1. Prove that from a function $f(t)$ calculated on the interval $[0, T]$ with time steps δt we can only obtain a spectral analysis in the frequency range $[-\pi/\delta t, \pi/\delta t]$ with a resolution $2\pi/T$.

   Hint: Try the two limits separately:

   i) Consider a continuous function defined on a finite time interval $[-T/2, T/2]$ – the time shift simplifies the calculation. The Fourier transform on this finite interval is defined as:

   $$\tilde{f}^T(\omega) = \int_{-T/2}^{T/2} \mathrm{d}t\, f(t) \mathrm{e}^{i\omega t}$$

   Take for example $f(t) = a_1 \mathrm{e}^{i\omega_1 t} + a_2 \mathrm{e}^{i\omega_2 t}$ with two definite Fourier components. Study under which condition on T one distinguishes the ω_1 from the ω_2 component in the Fourier transform of $\tilde{f}^T$ over the time interval $[-T/2, T/2]$.

   ii) Calculate now the discrete fourier transform

   $$\tilde{f}^{\delta t}(\omega) = \sum_{n=1}^{\infty} \mathrm{e}^{in\,\delta t\,\omega} f(n\,\delta t)$$

   of a generic function $f(t)$. Prove that $\tilde{f}^{\delta t}(\omega) = \tilde{f}^{\delta t}(\omega + 2\pi/\delta t)$. What happens if $f(t) = \mathrm{e}^{i\omega_1 t}$?

2. For the system introduced in the first exercise, verify numerically that the only spectral components in the evolution of the density matrix are at the Bohr frequencies.

3. Taking advantage of the result obtained at point 2.1 verify numerically that the calculation of the spectral components of the density matrix for the system introduced in the first exercise is most efficient if $\delta t \approx \hbar\pi/4|b|$ and the number of time steps $N_t \approx 2N$ where N is the number of sites in the ring.

Frohes Schaffen!