Density Matrix Theory

Lectures	Wed	11:15 - 12:45	PHY 2.0.31
	Thu	10:00 - 11:30	PHY 2.1.29
Exercises	Fri	14:00 - 15:45	PHY 9.1.10

Sheet 3

1. Eigenstates, pure states, mixed states

Let us consider a quantum ring described by the Hamiltonian:

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

where $c_\alpha^\dagger$ creates a (spinless) particle on the α site and we impose periodic boundary conditions: $c_{N+1} = c_1$. The single particle energy eigenvectors $\{|\ell\rangle\}$ of the system can be written as:

$$|\ell\rangle \equiv c_\ell^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha=1}^{N} e^{i\ell \frac{2\pi}{N}\alpha} c_\alpha^\dagger |0\rangle,$$

where $\ell = 0 \ldots N-1$ and $|0\rangle$ is the vacuum state. The corresponding eigenvalue is $E_\ell = \varepsilon + 2b\cos\left(\frac{2\pi}{N}\ell\right)$.

1. Calculate the time evolution of the eigenvector $|\ell\rangle$ and prove that after a time interval

   $$T = [\varepsilon + 2b\cos(\tfrac{2\pi\ell}{N})]^{-1} \tfrac{2\pi\ell}{N}\hbar$$

   the vector is rotated in space of an angle $2\pi/N$ with respect of the initial vector. Is this rotation physical? What happens if we measure the energy starting from another reference point?
   (Hint: Due to the geometry of the system, a rotation in space of an angle $2\pi/N$ brings the position basis vector $|\alpha\rangle$ into the vector $|\alpha+1\rangle$).

2. Calculate now the time evolution of the pure state $|\ell\rangle\langle\ell|$. Prove that the density matrix is stationary in whatever basis. Comment the result.

3. Consider now the time evolution of the pure state $|\psi\rangle\langle\psi|$, where $|\psi\rangle = a_1|\ell_1\rangle + a_2|\ell_2\rangle$ with $\ell_1 \neq \ell_2$ and $|a_1|^2 + |a_2|^2 = 1$. Prove that this time the density matrix is evolving in time if $E_{\ell_1} \neq E_{\ell_2}$. Prove that the evolution, at least at finite time intervals can be interpreted as a rotation in space. Find the period of the rotation.

4. Finally consider as an initial condition a mixed state of energy eigenstates: $\rho(t=0) = \sum_{\ell=0}^{N-1} p_\ell |\ell\rangle\langle\ell|$, with $\sum_\ell p_\ell = 1$. Is this density matrix evolving in time?

5. Visualize all the results obtained in the previous points by using the time evolution code developed for the previous exercise sheet and extending it to the generic N site system.

Bitte, wenden

2. Reduced density matrix of a spin chain

Consider a closed spin-1/2 chain, described by the Hamiltonian

$$\hat{H} = \sum_{\alpha=1}^{N} J\hat{S}_\alpha \cdot \hat{S}_{\alpha+1}$$

with periodic boundary conditions $\hat{S}_{N+1} \equiv \hat{S}_1$, and the i^{th} component (*i.e.* $i = x, y, z$) of the spin operator reads $\hat{S}^{(i)}_\alpha := \frac{\hbar}{2}\sum_{\tau\tau'} c^\dagger_{\alpha\tau}\sigma^{(i)}_{\tau\tau'}c_{\alpha\tau'}$ where $c^\dagger_{\alpha\tau}$ creates an electron with spin τ on site α and $\sigma^{(i)}_{\tau\tau'}$ is the i^{th} Pauli matrix. Assume that the chain is prepared, at time $t = 0$ into the initial state:

$$|\phi(0)\rangle = c^\dagger_{1\uparrow}\prod_{\alpha=2}^{N} c^\dagger_{\alpha\downarrow}|\varnothing\rangle.$$

1. Prove that $|\phi(t)\rangle$ can only be found in the N dimensional Hilbert space spanned by the vectors:

   $$|\alpha\rangle = \hat{S}^+_\alpha \prod_{\beta=1}^{N} c^\dagger_{\beta\downarrow}|\varnothing\rangle$$

   where $\alpha = 1, \ldots, N$ and $\hat{S}^+_\alpha = \hat{S}^x_\alpha + i\hat{S}^y_\alpha$.

2. Find the eigenvalues and eigenvectors of $\hat{H}$ within the Hilbert space identified in the previous point.

3. Calculate the time evolution of the full density operator $|\phi(t)\rangle\langle\phi(t)|$ and, by partial tracing over the degree of freedom of the sites $2, \ldots, N$, give the time evolution of the reduced density operator of the site 1.

   Hint: You should obtain an expression like

   $$\hat{\rho}_{\text{red}}(t) = P_\uparrow(t)|\uparrow\rangle\langle\uparrow| + P_\downarrow(t)|\downarrow\rangle\langle\downarrow|$$

4. Perform the limit $N \to \infty$ of the previous result, and comment on the physical meaning of the stationary limit.

5. Repeat the same operations of the previous points, but now consider the initial condition

   $$|\phi(0)\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\uparrow} + c^\dagger_{1\downarrow})\prod_{\alpha=2}^{N} c^\dagger_{\alpha\downarrow}|\varnothing\rangle.$$

   Which is the stationary state of the reduced density matrix in the limit $N \to \infty$?

Frohes Schaffen!