Density Matrix Theory

Lectures	Tue	12:00 - 13:30	PHY 5.0.20
	Thu	10:15 - 12:00	PHY 9.1.09
Exercises	Fri	10:15 - 12:00	PHY 5.0.21

Sheet 1

1. Statistical mixture of non-orthogonal states

Prove that the relation

$$\mathrm{Tr}\hat{\rho}^2 \leqslant (\mathrm{Tr}\hat{\rho})^2 \tag{1}$$

holds true for a generic density operator $\hat{\rho} = \sum_n w_n |\psi_n\rangle\langle\psi_n|$ where $\sum_n w_n = 1$ and $\{|\psi_n\rangle\}$ is a set of normalized but, in general,*not* mutually orthogonal state vectors. Moreover, prove that the equal sign in (1) only holds for pure states.

2. Pure vs. mixed states

Consider the two orbital interacting model for a molecule described by the following Hamiltonian:

$$H = \varepsilon\hat{N} + J\hat{S}_1 \cdot \hat{S}_2 \tag{2}$$

where $\hat{N} = \hat{N}_1 + \hat{N}_2$ with $\hat{N}_i = \sum_\tau c^\dagger_{i\tau} c_{i\tau}$ counts the number of electrons in the system and $c_{i\tau}$ destroys an electron of spin τ and orbital i. Moreover $\hat{S}_{i,\alpha}$ is the component $\alpha = x, y, z$ of the spin vector operator associated to the orbital i.

a) Consider the set of operators $\mathcal{S} = \{\hat{N}_1, \hat{N}_2, \hat{S}^2, \hat{S}_z\}$, where $\hat{S}^2 = (\hat{S}_1 + \hat{S}_2) \cdot (\hat{S}_1 + \hat{S}_2)$ and, correspondingly $\hat{S}_z = \hat{S}_{1,z} + \hat{S}_{2,z}$ is the z component of the total spin operator. Prove that $\mathcal{S}$ is a complete set of operators for the entire Fock space of the system.

b) Prove that the measurement of $\langle\hat{N}_1\rangle = 2$ and $\langle\hat{N}_2\rangle = 0$ gives full knowledge over the state of the molecule.

c) How many paramenters (*i.e.* observables) are needed, in general, to fully characterize the quantum state of the molecule? How does this number change if we measure $\langle\hat{N}_1\rangle = \langle\hat{N}_2\rangle = 1$? Why? What about the case in which the previous result in the measurement of the particle numbers is obtained *without* any dispersion?

Frohes Schaffen!