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 1

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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 if and only if $\hat{\rho}$ describes a pure state.

Hint: To prove relation (1), you can use the Cauchy-Schwarz inequality which states:

$$|\langle a|b\rangle|^2 \leq \langle a|a\rangle \cdot \langle b|b\rangle \tag{2}$$

for any generic pair of vectors $|a\rangle$ and $|b\rangle$.

2. Pure vs. mixed states

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

$$\hat{H} = \varepsilon \hat{N} + J\hat{S}_1 \cdot \hat{S}_2 \tag{3}$$

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 $\hat{S}_{i,\alpha} = \frac{\hbar}{2} \sum_{\tau\tau'} c^\dagger_{i\tau} \sigma^{(\alpha)}_{\tau\tau'} c_{i\tau'}$ is the component $\alpha = x, y, z$ of the spin vector operator associated to the orbital i. The Pauli matrices are denoted by $\sigma^{(\alpha)}$.

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. Verify that $\mathcal{S}$ is a complete set of operators: i.e. the common eigenvector associated to a string of eigenvalues for all the operators in $\mathcal{S}$ is unique.

b) List the eigenvalues of $\hat{H}$ with the associated eigenvectors. Is $\mathcal{S}' = \{\mathcal{S}, \hat{H}\}$ complete? Give an alternative complete set of operators for the system.

c) 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.

d) 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!