

1. Pure ensemble

The concept of pure ensemble in a nutshell: In a pure ensemble every state is the same, thus statistical mechanics of such an ensemble reduces to ordinary quantum mechanics.

- a) Show that the relation $\rho^2 = \rho$ holds for the density operator of a pure ensemble and thus $\text{Tr}(\rho^2) = 1$.
- b) Show that the corresponding matrix representation is given by a matrix where one of the diagonal elements is 1 and the rest are zero. Is this always true?

2. Mixed ensemble

Suppose we have a mixed ensemble of spin- $\frac{1}{2}$ particles with $\frac{1}{3}$ of the ensemble in the state $|S_z; \uparrow\rangle$ and the rest in the state $|S_z; \downarrow\rangle$

- a) Find a matrix representation for the density operator in the $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$ basis.
- b) Calculate the ensemble averages of operators S_x , S_y and S_z in this ensemble. Calculate the same averages in an unpolarized ensemble (completely mixed ensemble) for which the density operator reads:

$$\rho = \frac{1}{2} (|S_z; \uparrow\rangle \langle S_z; \uparrow| + |S_z; \downarrow\rangle \langle S_z; \downarrow|).$$

Comment your findings.

- c) In spherical coordinates the unit vector $\hat{\mathbf{n}}$ can be written

$$\hat{\mathbf{n}} = \sin \theta \cos \phi \hat{\mathbf{i}} + \sin \theta \sin \phi \hat{\mathbf{j}} + \cos \theta \hat{\mathbf{k}}.$$

Find $[\mathbf{S} \cdot \hat{\mathbf{n}}]$ for an arbitrary axis $\hat{\mathbf{n}}$ for the two ensembles considered above, where notation $[A]$ means ensemble average of operator A . Verbalize your results.

3. Time evolution operator

Derive the formal solutions of the Schrödinger equation for time-evolution operator:

$$i\hbar \frac{\partial}{\partial t} \mathcal{U}(t, t_0) = H \mathcal{U}(t, t_0)$$

in the three cases considered during lectures:

- a) Hamiltonian H does not depend on time.
- b) Hamiltonian H depends on time but the operators $H(t')$ and $H(t'')$ corresponding to different moments of time commute.
- c) Hamiltonians H evaluated at different moments of time do not commute.

4. A time dependent quantum system

Consider a physical system whose three-dimensional state space is spanned by the orthonormal basis formed by $|u_1\rangle$, $|u_2\rangle$ and $|u_3\rangle$. In this basis, the Hamiltonian H of the system and two observables A and B have matrix representations

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad A = \hbar\omega_0 \begin{pmatrix} a & 0 & 0 \\ 0 & 0 & a \\ 0 & a & 0 \end{pmatrix}, \quad B = \hbar\omega_0 \begin{pmatrix} 0 & b & 0 \\ b & 0 & 0 \\ 0 & 0 & b \end{pmatrix},$$

where all constants are positive and real. The initial state is

$$|\alpha, t_0 = 0\rangle = \frac{1}{\sqrt{2}} |u_1\rangle + \frac{1}{2} |u_2\rangle + \frac{1}{2} |u_3\rangle.$$

- The energy of the system is measured at $t = 0$. What energies with which probabilities can be found? What are the mean energy and variance (dispersion) of energy?
- If A is measured at $t = 0$, what values can be found and with which probabilities? What is the state vector immediately after the measurement?
- What is $|\alpha, t_0, t\rangle$?
- Calculate the expectation values of A and B as a function of time. Can you comment something?
- What results can be obtained if A is measured at time t . How about B ? Again, try to verbalize your results?

5. Non-compatible operators and the degeneracy of energy eigenstates

Two observables A_1 and A_2 which do not involve time explicitly, are known NOT to commute,

$$[A_1, A_2] \neq 0.$$

However, both of them commute with the Hamiltonian

$$[A_1, H] = 0, \quad [A_2, H] = 0.$$

Show that the energy eigenstates are, in general, degenerate. Are there exceptions? For example, you can consider the central-force problem $H = \mathbf{p}^2/2m + V(r)$ with $A_1 = L_z$ and $A_2 = L_x$.