Übungen zur Quantenmechanik für LA und Nanoscience
Blatt 4 (für die Übungen in der Woche 13.-17.11.)

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1 Measurements in a three-dimensional Hilbert space

Consider the following three operators on a three-dimensional complex Hilbert space,

$$L_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad L_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

a) Consider the eigenbasis of L_z. What are the possible results if L_z is measured? Find $\langle L_x \rangle$, $\langle L_x^2 \rangle$, and ΔL_x in the state for which L_z has eigenvalue $+1$. (See last week's problem 4b) for the notation.)

b) Find the eigenvalues and the normalized eigenstates of L_x. Express the latter in the L_z-basis.

c) If the particle is in the state with $L_z = -1$ and L_x is measured, what are the possible outcomes and their probabilities?

d) Consider the normalized state

$$|\psi\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ \sqrt{2} \end{pmatrix}.$$

If L_x^2 is measured and the result $+1$ is obtained, what is the state after the measurement? How probable was this result? If L_z is measured, what are the outcomes and respective probabilities?

e) A particle is in a state for which the probabilities are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$, and $P(L_z = -1) = 1/4$. Convince yourself that the most general normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle .$$

In quantum mechanics, states that only differ by a phase are considered to be equivalent. Does this mean that the factors $e^{i\delta_i}$ in the expression above are irrelevant? (Calculate for example $P(L_x = 0)$.)

2 The density matrix

More common than single-particle systems in pure states $|\psi\rangle$ are ensembles of N systems, n_i of which are in the state $|i\rangle$. (For simplicity, we restrict ourselves to cases where $|i\rangle$ is an element of an orthonormal basis.) Such an ensemble is described by k states $|i\rangle = |1\rangle, |2\rangle, \ldots, |k\rangle$ and by k occupation numbers n_i $(i = 1, 2, \ldots, k)$. A convenient way to assemble all this information is the density matrix (which is really an operator that turns into a matrix once a basis is chosen),

$$\rho = \sum_i p_i |i\rangle\langle i| ,$$

where $p_i = n_i/N$ is the probability that a system picked randomly out of the ensemble is in the state $|i\rangle$. The single-particle systems considered up to now correspond to the situation of a *pure* ensemble in which all $p_i = 0$ except one. A general ensemble is *mixed*. In such an ensemble one considers *ensemble averages* of operators Ω, which are defined as

$$\langle \bar{\Omega} \rangle \equiv \sum_i p_i \langle i|\Omega|i\rangle \, .$$

The notation with the bar and the angular brackets indicates that two types of averages have been taken: a quantum average $\langle i|\Omega|i\rangle$ for each system in a given state $|i\rangle$, and a classical average over the systems in different states $|i\rangle$.

a) Define $\mathrm{tr}(\Omega\rho) \equiv \sum_j \langle j|\Omega\rho|j\rangle$. Show that $\langle \bar{\Omega} \rangle = \mathrm{tr}(\Omega\rho)$. (This demonstrates that ρ contains all the statistical information about the ensemble.)

b) Prove the following list of properties. Also give an interpretation and/or list immediate consequences where possible.

   i) $\rho^\dagger = \rho$.
   ii) $\mathrm{tr}\,\rho = 1$.
   iii) $\rho^2 = \rho$ for a pure ensemble.
   iv) $\rho = (1/k)\mathbb{1}$ for an ensemble uniformly distributed over k states. Here, $\mathbb{1}$ is the identity operator on the space spanned by these states.
   v) $\mathrm{tr}\,\rho^2 \leq 1$.

3 Time-evolution operator

In the lecture we will consider the so-called time-evolution operator. In an eigenbasis $\{|E\rangle\}$ of the Hamilton operator H it takes the form

$$U(t) = \sum_E |E\rangle\langle E| e^{-iEt/\hbar} \, .$$

Show that its general form, without reference to any basis, is given by $U(t) = e^{-iHt/\hbar}$.

4 Properties of the Dirac δ-function

Use the relation $\delta(ax) = \delta(x)/|a|$ to show that

$$\delta[f(x)] = \sum_{i=1}^{n} \frac{\delta(x - x_i)}{|df/dx|_{x=x_i}} \, ,$$

where $x_1, x_2, \ldots, x_n$ are the zeros of $f(x)$ (which we assume to be simple zeros).
Hint: Start from the integral

$$\int_{-\infty}^{+\infty} dx \, \delta[f(x)] g(x)$$

and rewrite it as a sum of n integrals, each of which is performed over an infinitesimal interval centered at one of the x_i. (What feature of the δ-function allows for this preliminary step?) Then expand $f(x)$ in a Taylor series and keep only the first nonzero contribution.