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Höhere Quantenmechanik
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Exercise sheet 3
(Submission date: Until 09.05.2022 12:00)

Exercise 1: time evolution *(5 Points)*

A particle with mass m is confined to a one-dimensional potential well of width a, and with infinite barriers, i.e. $0 < x < a$.

(i) Find the eigenfunctions and energies of the time-independent Schrödinger equation. *(2 Points)*

(ii) Suppose that at time $t = 0$ the particle is in the state described by the wave function

$$\Psi(x, t = 0) = \frac{1}{\sqrt{a}} \left[1 + 2\cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right).$$

Compute its time-evolved wave function at a generic time t. *(1 Point)*
Hint: use the information from the previous point

(iii) Compute the probability that the particle is at $x \geq a/2$ at time t. *(2 Points)*
Hint: $\int dx \sin(x)\sin(2x) = \frac{2}{3}\sin^3(x)$

Exercise 2: groups and representations *(6 Points)*

In mathematics, a group is a set of elements with a binary operation that fulfills certain properties. For simplicity, in this exercise we consider the case of finite discrete groups, where we can denote the set of elements as $\mathcal{G} = \{g_\alpha\}_{\alpha=1,\dots,N}$ (N being the total number of elements). The binary operation is indicated by $\circ$. The properties that define a group are the following

- *closure*: the set needs to be closed with respect to the operation. This means that the result of the application of $\circ$ between two elements of $\mathcal{G}$ is an elements of $\mathcal{G}$, i.e. $g_\alpha \circ g_\beta = g_\gamma$, $g_\alpha, g_\beta, g_\gamma \in \mathcal{G}$.
- *associativity*: the operation needs to be associative, i.e. $(g_\alpha \circ g_\beta) \circ g_\gamma = g_\alpha \circ (g_\beta \circ g_\gamma)$
- *existence of the identitiy element*: there exist an element $e \in \mathcal{G}$ such that $g_\alpha \circ e = e \circ g_\alpha = g_\alpha$
- *existence of the inverse*: for each element $g_\alpha \in \mathcal{G}$, there exist an inverse element $g_\alpha^{-1} \in \mathcal{G}$ such that $g_\alpha \circ g_\alpha^{-1} = g_\alpha^{-1} \circ g_\alpha = e$

When the operation $\circ$ is commutative, i.e. $g_\alpha \circ g_\beta = g_\beta \circ g_\alpha$, the group is said to be *Abelian*.

Groups are abstract concepts. To define them, we just need to specify the elements of $\mathcal{G}$ and how the operation connects them. *Representation theory* is the study of the concrete ways in which abstract groups can be realized. A representation is a mapping ρ from the group $\mathcal{G}$

(elements and operation) to a vector space V. For our practical purposes, representing a group means expressing its elements as matrices of a given dimension, $g \in \mathcal{G} \mapsto \rho(g) \in V$, and the operation among them as a matrix-matrix product (note: this explanation is a bit sloppy), such that $g_\alpha \circ g_\beta = g_\gamma \;\Rightarrow\; \rho(g_\alpha)\rho(g_\beta) = \rho(g_\gamma)$. The dimension of the representation is equal to the dimension of the vector space V (which can be a complex space, in general).

(i) We consider a group that contains two elements (among others), σ and τ. Its binary operation is denoted by $\circ$. The above elements satisfy the following properties

$$\sigma \circ \tau = \tau \circ \sigma \qquad \tau^2 = e \qquad \sigma^4 = e \tag{1}$$

Here, the powers denote a repeated application of the operation $\circ$ between identical elements, e.g. $\tau^3 = \tau \circ \tau \circ \tau$. The element e is the identity. Using σ, τ and e it is possible to construct all the inequivalent elements of the group by applying the operation $\circ$. Can you do it? How many are they? Is the group Abelian? *(1 Point)*

(ii) In the previous point, we gave an abstract definition of the group. Now we want to construct a representation ρ. Consider the matrices

$$\Sigma = \rho(\sigma) = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \qquad T = \rho(\tau) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad E = \rho(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Verify that ρ is a valid representation. Note: the operation $\circ$ is represented by the matrix product. *(1 Point)*

(iii) Representations of a group are not unique. This is exemplified by the fact that we can define a new representation ρ' for the group, i.e.

$$\Sigma' = \rho'(\sigma) = \begin{pmatrix} i & 0 \\ 1 & 1 \end{pmatrix} \qquad T' = \rho'(\tau) = \begin{pmatrix} -1 & 0 \\ i+1 & 1 \end{pmatrix} \quad \text{and} \quad E' = \rho'(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Prove that this is a valid representation. *(1 Point)*

(iv) So far we have constructed two-dimensional representations of the group (i.e., 2×2 matrices). We could also construct one-dimensional representations, i.e. represent the elements by scalars ("1×1 matrices"). The simplest example is the trivial representation, where each element of the group is represented by the number 1. This obviously satisfies the relations among the elements. Can you find another one-dimensional representation for the group of this exercise? *(1 Point)*

(v) We now want to give a physical interpretation of the group. Consider the planar molecule in Fig. 1. We have numbered its "arms". Our group is the group of symmetries of this molecule (the group is sometimes called C_{4h}). Indeed, we have a so-called C_4 rotation, i.e. a rotation of 90°, which transforms arm 1 into arm 2, arm 2 into arm 3, and so on. This corresponds to our element σ (after *four* rotations, we are back to the initial configuration). Another symmetry is the inversion with respect to the center of the molecule (i.e., the Cu atom). This operations transforms arm 1 into arm 3 (and viceversa), arm 2 into arm 4 (and viceversa). This corresponds to our element τ (*two* inversions bring us back to the initial configuration).

Does $\sigma \circ \tau = \tau \circ \sigma$ hold for these symmetry operations? Sketch an example to show that it holds. We can express the coordinates of the atoms in terms of the cartesian axes depicted in Fig. 1 (x parallel to arm 1 and y parallel to arm 2). Can you write down the 2×2 matrices which implement the symmetries in these coordinates? Are they a valid representation of our group? *(2 Points)*

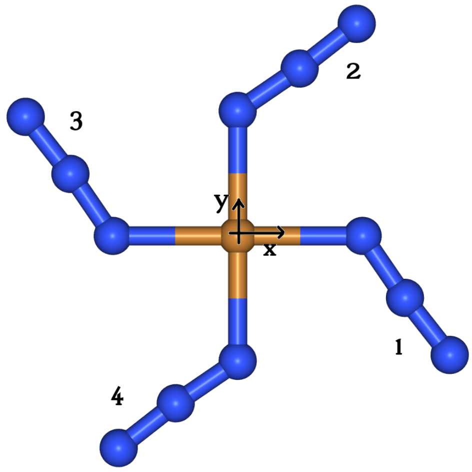

Figure 1: Tetraazidocopper(II). Orange and blue denote Cu and N atoms, respectively.

Exercise 3: spin-$\frac{1}{2}$ rotations *(4 Points)*

(i) Consider a particle with spin $\frac{1}{2}$. Rotate the wave function $|\phi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i\,|\downarrow\rangle)$ by 90° around the x-axis. *(1 Point)*

(ii) We now consider a system of two spin-$\frac{1}{2}$ particles. Show that the singlet wave function, $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, is invariant under generic global rotations (i.e. rotations of both spins). *(3 Points)*

Hint: As discussed in the notes, a generic rotation for a single spin can be written as a 2×2 unitary matrix with determinant 1. A possible parametrization of the matrix is

$$U = \begin{pmatrix} e^{i\delta}\cos(\gamma) & ie^{-i\phi}\sin(\gamma) \\ ie^{i\phi}\sin(\gamma) & e^{-i\delta}\cos(\gamma) \end{pmatrix}$$

For the system of two spins, we need to consider the global rotation, which can be written as $U \otimes U$, and apply it to the singlet state, $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle)$.

Exercise 4: translation operator *(5 Points)*

(i) Compute the commutator $[\mathbf{x}, U(a)]$ between the position operator $\mathbf{x}$ and the translation operator $U(a) = \exp\left(\frac{i}{\hbar}a\mathbf{p}\right)$ in one dimension. *(3 Points)*
Hint: first obtain the result of the commutator $[\mathbf{x}, \mathbf{p}^n]$ by induction ($n \in \mathbb{N}$).

(ii) If $\mathbf{x}|x'\rangle = x'|x'\rangle$, show that $U(a)|x'\rangle$ is still an eigenstate of $\mathbf{x}$. What is the corresponding eigenvalue? *(2 Points)*