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Exercise sheet 3 (Due: Monday October, 28th.)

3.1 Invariant subspaces and para-statistics

We have learned that identical particles are either bosons or fermions, where the former are associated to totally symmetric vectors, while the latter are associated to totally anti-symmetric vectors. Could one imagine something other than this? In this exercise we explore a theoretical alternative, sometimes referred to as para-statistics.

Suppose that we have a basis $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle\}$ of a three-dimensional single particle space. We furthermore have three indistinguishable particles that occupy these states. As in the lecture, we made use of the group of permutations, and here we need the group of permutations of three objects $S_3 = \{1, \pi_{12}, \pi_{23}, \pi_{31}, \pi_{123}, \pi_{132}\}$. Here π_{12} means the transposition between particles 1 and 2 (i.e., they are swapped), and analogous for π_{23} and π_{31}. The notation π_{123} means $1 \mapsto 2$, $2 \mapsto 3$, and $3 \mapsto 1$. Analogously π_{132} means $1 \to 3$, $3 \to 2$ and $2 \to 1$. In the two-line notation that we discussed in the lecture

$$\pi_{123} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \quad \pi_{132} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}.$$

Recall from the lecture that the action of π on a basis vector $|i_1, i_2, i_3\rangle$ is given by $\pi|i_1, i_2, i_3\rangle = |\pi(i_1), \pi(i_2), \pi(i_3)\rangle$. For example,

$$\pi_{12}|\alpha, \beta, \gamma\rangle = |\beta, \alpha, \gamma\rangle, \quad \pi_{123}|\alpha, \beta, \gamma\rangle = |\gamma, \alpha, \beta\rangle, \quad \pi_{132}|\alpha, \beta, \gamma\rangle = |\beta, \gamma, \alpha\rangle.$$

(a) We first want to determine the bosonic and the fermionic state vector, for the case where each single-particle state is occupied by precisely one particle. *Apply the symmetrization operator to $|\alpha, \beta, \gamma\rangle$ and normalize, in order to find the bosonic state vector. Apply the anti-symmetrization operator to $|\alpha, \beta, \gamma\rangle$ and normalize, in order to find the fermionic state vector.* **(3 points)**

When the six permutations $1, \pi_{12}, \pi_{23}, \pi_{31}, \pi_{123}, \pi_{132}$ act on the state $|\alpha, \beta, \gamma\rangle$, we obtain six orthonormal states that thus span a six-dimensional space. If the particles are indistinguishable, no experiment would be able to detect any difference between the elements of this space. The bosonic and fermionic vectors from (a) only take two of these dimensions, so there is still room for more. In the following we sha find another subspace that also is invariant under S_3.

(b) *Show that all elements of S_3 can be written as products of π_{12} and π_{31}.* **(2 points)**
Remark: The technical term is that π_{12} and π_{31} are generators of S_3.

Consider the two orthonormal vectors

$$|\psi_1\rangle = \frac{1}{\sqrt{12}}(2|\alpha, \beta, \gamma\rangle + 2|\beta, \alpha, \gamma\rangle - |\alpha, \gamma, \beta\rangle - |\gamma, \beta, \alpha\rangle - |\gamma, \alpha, \beta\rangle - |\beta, \gamma, \alpha\rangle),$$
$$|\psi_2\rangle = \frac{1}{2}(-|\alpha, \gamma, \beta\rangle + |\gamma, \beta, \alpha\rangle + |\gamma, \alpha, \beta\rangle - |\beta, \gamma, \alpha\rangle).$$

(c) *Show that the action of π_{12} on these vectors is given by $\pi_{12}|\psi_1\rangle = |\psi_1\rangle$, $\pi_{12}|\psi_2\rangle = -|\psi_2\rangle$. Argue that this means that $\pi_{12}|v\rangle \in \mathcal{V}$ for all $|v\rangle \in \mathcal{V} = \mathrm{Sp}\{|\psi_1\rangle, |\psi_2\rangle\}$.* In other words, show that the space spanned by $|\psi_1\rangle, |\psi_2\rangle$ is left invariant by π_{12}. **(3 points)**

(d) *Show that $\mathcal{V}$ also is invariant under π_{31}.*
Combine this result with (a) and (c) to prove that $\mathcal{V}$ is invariant under all of S_3.
Hint: Show that $\pi_{31}|\psi_1\rangle$ and $\pi_{31}|\psi_2\rangle$ are linear combinations of $|\psi_1\rangle$ and $|\psi_2\rangle$. **(4 points)**

Remark on the whole exercise: This exercise shows that there exist additional invariant subspaces, apart from the symmetric and anti-symmetric ones. One could imagine that state vectors of identical particles would be elements of such subspaces, thus obeying para-statistics, rather than Bose- or Fermi-statistics. However, it seems that nature does not favour such alternatives.

3.2 Energy spectrum for identical particles

In the lecture we discussed how the anti-symmetry of the wave-function of fermions underpins the electronic structure of atoms. In this exercise, we explore the effect of symmetry and anti-symmetry on the energy spectrum of a simple model of a diatomic molecule.

Suppose that we have two identical particles of mass m on a line, and that these interact via a harmonic potential, such that the Hamiltonian is $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{k}{2}(x_1 - x_2)^2$. As you may recall, it is useful to change to the center of mass coordinate $R = (mx_1+mx_2)/(2m) = \frac{1}{2}(x_1+x_2)$ and the relative coordinate $r = x_1 - x_2$. By separation of variables, the eigenfunctions of H can be written $\psi_{p,n}(R,r) = e^{ipR}\phi_n(r)$, where ϕ_n for $n = 0, 1, 2, \ldots$ are the solutions to the harmonic oscillator $H' = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{k}{2}r^2$, with the reduced mass $\mu = m/2$.

(a) How does r and R transform under the exchange of particles? What can we conclude concerning the symmetry or anti-symmetry of the factor e^{ipR}? Argue that it is only $\phi_n(r)$ that determines whether $\psi_{p,n}(R,r)$ is symmetric or anti-symmetric under particle exchange. **(2 points)**

(b) For which $n = 0, 1, 2, \ldots$ does ϕ_n correspond to a solution that is symmetric under permutation of particles 1 and 2, and for which n are they anti-symmetric? If these particles have no additional degrees of freedom, what would be the spectrum be for two identical bosons, and what would it be for two identical fermions? Ignore the center of mass motion, and express the spectrum in terms of m and k. **(2 points)**

(c) Suppose now that the two particles in addition have a spin degree of freedom, and more precisely that they are spin-half fermions. What is the spectrum, and what are the degeneracies? (Do again ignore the center of mass motion.) What is the lowest energy that the system can have if the total spin is restricted to be in a spin-singlet state? What is the lowest energy if it is restricted to a spin triplet? **(4 points)**

Remark: The Hamiltonian in this example has no explicit dependence on the spin. Nevertheless, the total energy depends on the spin-state. This may at first sight seem perplexing, but is due to the restriction of the state space imposed by the anti-symmetrization (or symmetrization). A striking example of this is the hydrogen molecule, H_2. The proton is a spin-half fermion, and thus the two protons can either be in a nuclear spin singlet state (parahydrogen) or in a nuclear spin triplet (orthohydrogen). Apart from the nuclear spin, the two protons can also orbit each other, and much analogous to this exercise, it turns out that the nuclear spin state affects the allowed orbital states, which leads to a different ground state energy for ortho- and parahydrogen. In the production of liquid hydrogen one often uses a catalyst to speed the conversion to the lowest energy state.