Problem 4.1: Representations of the Symmetric Group

ID: ex_representations_of_the_symmetric_group:aqt2223

Learning objective

Here you verify some of the statements from the lecture on representations of the symmetric group in the many-particle Hilbert space. In particular, you study the properties of the symmetrizer and antisymmetrizer to familiarize yourself with these rather abstract operators.

First, we consider the Hilbert space $H^n = L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3)$ of $n$ (distinguishable) particles with position basis $|x_1, \ldots, x_n\rangle$ in $\mathbb{R}^3$. The representation of the permutation group $S_n$ is defined by

$$U_\pi |x_1, \ldots, x_n\rangle := |x_{\pi 1}, \ldots, x_{\pi n}\rangle$$

for all permutations $\pi \in S_n$.

a) Show that $U_\pi$ defines a representation of $S_n$ on $H^n$, i.e., show that

$$U_\pi \cdot U_\rho = U_{\pi \rho}$$

for all $\pi, \rho \in S_n$. Here, “·” denotes the multiplication of operators on $H^n$ and $\pi \rho$ is the group multiplication on $S_n$ (the concatenation of permutations).

b) Prove that $U_\pi$ is a unitary representation, i.e., $U_\pi^\dagger = U_\pi^{-1}$.

c) Show that $U_\pi$ acts on the wave functions $\Psi(x_1, \ldots, x_n) = \langle x_1, \ldots, x_n | \Psi \rangle$ as defined in the lecture, i.e.,

$$U_\pi \Psi(x_1, \ldots, x_n) = \Psi\left(x_{\pi^{-1} 1}, \ldots, x_{\pi^{-1} n}\right)$$

with $\pi^{-1}$ the inverse of $\pi$ in $S_n$.

Let us now focus on a finite-dimensional single-particle Hilbert space $\mathcal{H} \simeq \mathbb{C}^d$ (imagine a particle that hops on a lattice with $d$ sites so that its position is discrete, $x \in \{1, \ldots, d\}$). The Hilbert space of $n$ particles $\mathcal{H}_n = \mathbb{C}^d \otimes \cdots \otimes \mathbb{C}^d$ is then $\dim \mathcal{H}_n = d^n$ dimensional.

The representation of permutations is given by Eq. (1) where now $x_i \in \{1, \ldots, d\}$ with the standard basis $|x_1, \ldots, x_n\rangle$ such that $\langle x_1, \ldots, x_n | y_1, \ldots, y_n \rangle = \delta_{x_1,y_1} \cdots \delta_{x_n,y_n}$.

As in the lecture, define the (anti-)symmetrizer $S(A)$ as

$$S := \frac{1}{n!} \sum_{\pi \in S_n} U_\pi \quad \text{and} \quad A := \frac{1}{n!} \sum_{\pi \in S_n} (-1)^\pi U_\pi$$

and the (anti-)symmetric subspaces as $\mathcal{H}_s = \{ S | \Psi \rangle \mid | \Psi \rangle \in \mathcal{H}^n \}$ and $\mathcal{H}_a = \{ A | \Psi \rangle \mid | \Psi \rangle \in \mathcal{H}^n \}$, respectively.
d) Prove that $S$ and $A$ are self-adjoint projectors, i.e., show that $S^\dagger = S$ and $S^2 = S$ (and the same for $A$).

**Hint:** Use the results from a) and b) and that $S_n$ is a group.

*e*) Show that $\dim \mathcal{H}_n = \binom{d}{n}$. What happens for $n > d$?

*f*) Similarly, show that $\dim \mathcal{H}_s = \binom{n+d-1}{d-1}$. What happens now for $n > d$?

**Hint:** How can you describe basis states in $\mathcal{H}_s$? Use combinatorial arguments to count them by means of $d-1$ “separators” that define $d$ “buckets.”

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**Problem 4.2: Identical Fermions in a Potential Well**

**Learning objective**

In the lecture you learned that the wave function of multiple fermions must be antisymmetric under the exchange of particles. Here you study the consequences of this rule by means of a simple toy model. In particular, you elaborate on the consequences of the antisymmetry in the presence of interactions between the fermions.

We consider two identical spin-$1/2$ fermions in a one-dimensional potential given by

$$V(x) = \begin{cases} 
0 & |x| \leq 1 \\
\infty & \text{otherwise}
\end{cases}$$  

(5)

The (dimensionless) single-particle Hamiltonian for the $i$th particle is given by

$$H^{(i)} = -\frac{1}{2} \partial^2_{x_i} + V(x_i).$$  

(6)

\[ \text{a) Explain why we can treat the orbital motion and the spin dynamics separately, that is, explain why we can write the single-particle eigenstates as a product of orbital- and spin wave functions. Write down the orbital wave functions and eigenenergies of the two single-particle eigenstates that are lowest in energy.} \]

\[ \text{b) Determine the ground state and the ground state energy of a two-fermion system with Hamiltonian } H = \sum_{i=1}^2 H^{(i)} \text{ in the following two cases:} \]

\[ \text{i. For a spin state that is antisymmetric under exchange of the two fermions, i.e., the singlet state } (|↑↓⟩ - |↓↑⟩)/\sqrt{2}. \]

\[ \text{ii. For a spin state that is symmetric under exchange of the two fermions, i.e., one of the triplet states } |↑↑⟩, |↓↓⟩ \text{ or } (|↑↓⟩ + |↓↑⟩)/\sqrt{2}. \]

\[ \text{c) Examine the influence of a contact-interaction between the two fermions which is described by the interaction potential } \lambda \delta(x_1 - x_2) \text{ with strength } \lambda \in \mathbb{R}. \text{ This end, calculate the energy correction in first order perturbation theory (assuming } |\lambda| \ll 1 \text{) for both the singlet state and the triplet states. Explain why the perturbative result for the triplet states is correct for arbitrary } \lambda. \]
Problem 4.3: Gross-Pitaevskii Equation

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**Learning objective**

Here we switch to identical bosons and determine the ground state of the system. Furthermore, the effect of weak interactions between the particles is studied approximately by means of a variational principle leading to the so-called Gross-Pitaevskii equation.

Consider \( N \) non-interacting bosons of mass \( m \) in a one-dimensional harmonic trap \( U_{\text{trap}}(x) = \frac{1}{2}m \omega^2 x^2 \).

a) Write down the ground state wave function for \( N \) bosons. What is the generalization to an arbitrary potential \( U(x) \) with the single-particle ground state wave function \( \phi_0(x) \)?

b) Now introduce a contact interaction of the form \( V(x_i - x_j) = V_0 \delta(x_i - x_j) \) between the particles. The Hamiltonian of this system is given by

\[
H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + U(x_i) \right) + V_0 \sum_{i<j} \delta(x_i - x_j).
\]

Write down the expectation value of this Hamiltonian with respect to the ground state wave function of the non-interacting system for an arbitrary external potential \( U(x) \) as calculated in a).

c) We treat the system by a variational principle where we approximate the ground state by a product wave function that minimizes the energy expectation value of \( H \) (this ansatz is known as Hartree-Fock approximation; the result of this minimization procedure is an exact eigenstate only for \( V_0 = 0 \), i.e., non-interacting bosons). Our variational parameter is the rescaled single-particle wave function \( \psi(x) \) defined as

\[
\psi(x) = \sqrt{N} \phi_0(x).
\]

The solution of the variational principle \( \psi(x) \) will differ from the single-particle ground state wave function of non-interacting bosons due to the interaction between the particles.

Show that the variational principle that minimizes the energy expectation value calculated in b) leads to the Gross-Pitaevskii equation

\[
\mu \psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + U(x) \psi(x) + V_0 |\psi(x)|^2 \psi(x)
\]

with the chemical potential \( \mu \). Note the non-linearity due to the interaction \( V_0 \! \).

**Hints:**

- Using the expression calculated in b), neglect all terms of order \( 1/N \) and treat the expectation value as a functional of the complex-valued function \( \psi(x) \). The result should read

\[
E[\psi, \psi^*] = \int dx \left( \frac{\hbar^2}{2m} |\partial_x \psi(x)|^2 + U(x) |\psi(x)|^2 + \frac{1}{2} V_0 |\psi(x)|^4 \right).
\]
• Minimize this functional with respect to $\psi(x)$ and $\psi^*(x)$ with the constraint

$$N = \int dx |\psi(x)|^2.$$  \hspace{1cm} (11)

This constraint can be taken into account by the method of Lagrange multipliers where the chemical potential $\mu$ is the Lagrangian multiplier that fixes the particle number (11).