Prof. Dr. Hans-Peter Büchler
Institute for Theoretical Physics III, University of Stuttgart

November 10th, 2022
WS 2022/23

Problem 4.1: Representations of the Symmetric Group

[**Oral** | 4 (+3 bonus) pt(s)]

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 $\mathcal{H}^n = L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3)$ 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

$$U_\pi |x_1, \ldots, x_n\rangle := |x_{\pi_1}, \ldots, x_{\pi_n}\rangle \tag{1}$$

for all permutations $\pi \in S_n$.

a) Show that U_π defines a representation of S_n on $\mathcal{H}^n$, i.e., show that **1**pt(s)

$$U_\pi \cdot U_\rho = U_{\pi\rho} \tag{2}$$

for all $\pi, \rho \in S_n$. Here, "$\cdot$" denotes the multiplication of operators on $\mathcal{H}^n$ and $\pi\rho$ is the group multiplication on S_n (the concatenation of permutations).

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

c) Show that U_π 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., **1**pt(s)

$$U_\pi \Psi(x_1, \ldots, x_n) = \Psi\left(x_{\pi_1^{-1}}, \ldots, x_{\pi_n^{-1}}\right) \tag{3}$$

with π^{-1} the inverse of π 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 $\langle x_1, \ldots, x_n|y_1, \ldots, y_n\rangle = \delta_{x_1,y_1} \ldots \delta_{x_n,y_n}$.

As in the lecture, define the (anti-)symmetrizer $\mathcal{S}$ ($\mathcal{A}$) as

$$\mathcal{S} := \frac{1}{n!} \sum_{\pi \in S_n} U_\pi \quad \text{and} \quad \mathcal{A} := \frac{1}{n!} \sum_{\pi \in S_n} (-1)^\pi U_\pi \tag{4}$$

and the (anti-)symmetric subspaces as $\mathcal{H}_s = \{\mathcal{S}|\Psi\rangle \mid |\Psi\rangle \in \mathcal{H}^n\}$ and $\mathcal{H}_a = \{\mathcal{A}|\Psi\rangle \mid |\Psi\rangle \in \mathcal{H}^n\}$, respectively.

d) Prove that $\mathcal{S}$ and $\mathcal{A}$ are self-adjoint projectors, i.e., show that $\mathcal{S}^\dagger = \mathcal{S}$ and $\mathcal{S}^2 = \mathcal{S}$ (and the same for $\mathcal{A}$). **1pt(s)**

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

*e) Show that $\dim \mathcal{H}_a = \binom{d}{n}$. What happens for $n > d$? **+1pt(s)**

*f) Similarly, show that $\dim \mathcal{H}_s = \binom{n+d-1}{d-1}$. What happens now for $n > d$? **+2pt(s)**

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."

Problem 4.2: Identical Fermions in a Potential Well

[**Written** | 3 pt(s)]

ID: ex_identical_fermions_in_a_potential_well:aqt2223

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

$$V(x) = \begin{cases} 0 & |x| \leq 1 \\ \infty & \text{otherwise}\,. \end{cases} \tag{5}$$

The (dimensionless) single-particle Hamiltonian for the ith particle is given by

$$H^{(i)} = -\frac{1}{2}\partial_{x_i}^2 + V(x_i)\,. \tag{6}$$

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. **1pt(s)**

Write down the orbital wave functions and eigenenergies of the two single-particle eigenstates that are lowest in energy.

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

i. For a spin state that is *antisymmetric* under exchange of the two fermions, i.e., the singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$.

ii. For a spin state that is *symmetric* under exchange of the two fermions, i.e., one of the triplet states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ or $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$.

c) Examine the influence of a contact-interaction between the two fermions which is described by the interaction potential $\lambda\,\delta(x_1 - x_2)$ with strength $\lambda \in \mathbb{R}$. To this end, calculate the energy correction in first order perturbation theory (assuming $|\lambda| \ll 1$) for both the singlet state and the triplet states. **1pt(s)**

Explain why the perturbative result for the triplet states is correct for arbitrary λ.

Problem 4.3: Gross-Pitaevskii Equation

[Oral | 3 pt(s)]

ID: ex_gross_pitaevskii_equation:aqt2223

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 $\phi_0(x)$? **1** pt(s)

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 **1** pt(s)

$$H = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + U(x_i)\right) + V_0\sum_{i<j}\delta(x_i - x_j)\,. \tag{7}$$

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 **1** pt(s)

$$\psi(x) = \sqrt{N}\phi_0(x)\,. \tag{8}$$

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

$$\mu\psi(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x) + U(x)\psi(x) + V_0|\psi(x)|^2\psi(x) \tag{9}$$

with the chemical potential μ. 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

$$E[\psi,\psi^*] = \int dx\,\left(\frac{\hbar^2}{2m}|\partial_x\psi(x)|^2 + U(x)|\psi(x)|^2 + \frac{1}{2}V_0|\psi(x)|^4\right)\,. \tag{10}$$

- Minimize this functional with respect to $\psi(x)$ and $\psi^*(x)$ with the constraint

$$N = \int dx\, |\psi(x)|^2 \,. \tag{11}$$

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