Introduction to computational quantum mechanics

Lecture 3: The Pauli principle and many-body Hilbert space

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Seminar series in quantum mechanics at CMA
Fall 2009
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Tensor product spaces

Configuration space and identical particles

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A note on tensor products of Hilbert spaces

- Let $\mathcal{H}_i$, $i = 1, 2$ be Hilbert spaces, with bases $\{\phi_{i,n}\}_n$, $i = 1, 2$.
- The space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined by

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \text{span} \left\{ \phi_{1,n_1} \otimes \phi_{2,n_2} \in \mathcal{H}_1 \times \mathcal{H}_2 \right\}$$

- Closure with respect to inner product:

$$\langle (\psi_1 \otimes \psi_2) | (\phi_1 \otimes \phi_2) \rangle := \langle \psi_1 | \phi_1 \rangle_1 \langle \psi_2 | \phi_2 \rangle_2.$$ 

- Examples:

$$L^2(\mathbb{R}^2) = L^2(\mathbb{R}) \otimes L^2(\mathbb{R}).$$

$$\mathbb{C}^{n^2} = \mathbb{C}^{n} \otimes \mathbb{C}^{n}.$$
Example of tensor product space

- The space \( L^2(0, 1) \) has an ONB \( \{ \phi_n \} \) where

\[
\phi_n(x) = \sqrt{2} \sin(n\pi x), \quad n = 1, 2, \ldots.
\]

- Forming the tensor products \( \Phi_{n_1, n_2}(x_1, x_2) \) we get

\[
\Phi_{n_1, n_2}(x_1, x_2) = (\phi_{n_1} \otimes \phi_{n_2})(x_1, x_2) = 2 \sin(n_1 \pi x_1) \sin(x_2 \pi x_2).
\]

- These \( \Phi_{n_1, n_2} \) form a basis for \( L^2(0, 1) \otimes L^2(0, 1) = L^2([0, 1]) \).
Vectors in product spaces

- Expansion in product basis:

\[ \Psi = \sum_{n_1,n_2} c_{n_1,n_2} \Phi_{n_1,n_2} \]

- By constructing a bijective map \( I : \mathbb{N}^2 \rightarrow \mathbb{N} \), we see that this is no different than ordinary basis expansions.

\[ \Psi = \sum_{\alpha} c_{I^{-1}(\alpha)} \Phi_{I^{-1}(\alpha)}, \quad \alpha = I(n_1,n_2) \]

- We typically abuse notation here and write \( c_\alpha = c_{n_1,n_2} \) etc, as there is usually no danger of confusion. Example of a map \( I \):

![Diagram of a map I]
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For a classical system, the \textit{configuration space} $\mathbb{X}$ is the space of configurations, i.e., the set of possible positions $x$ for the system. A manifold.

The quantum mechanical Hilbert space for the quantum version of the system is then

\[ \mathcal{H} = L^2(\mathbb{X}) \]

In QM, $\mathbb{X}$ contains additional \textit{discrete degrees of freedom}: for example spin. This has no classical analogue.
Spin/discrete degrees of freedom

- Consider a finite, discrete set $S$:
  $$S = \{s_1, s_2, \ldots, s_{|S|}\}$$

- Consider the manifold
  $$Y = X \times S.$$
Adding discrete degrees of freedom

- $S$ is equipped with counting measure, so that
  \[ L^2(S) = \mathbb{C}^{|S|}. \]

- The space $L^2(\mathbb{X} \times S)$ becomes
  \[ L^2(\mathbb{X} \times S) = L^2(\mathbb{X}) \otimes \mathbb{C}^{|S|} \cong L^2(\mathbb{X})^{|S|}. \]

- $\Psi$ is a function of $x \in \mathbb{X}$ and $s \in S$ simultaneously:
  \[ \Psi = \Psi(x, s) \rightsquigarrow \Psi_s(x) \]

That is, $\Psi \in L^2(\mathbb{X} \times S)$ is essentially $|S|$ component functions
$\Psi_s \in L^2(\mathbb{X})$, $s \in S$.

- The inner product is
  \[ \langle \Psi | \Phi \rangle = \sum_s \langle \Psi_s | \Phi_s \rangle. \]

- “Some degrees of freedom are continuous (which we integrate over), and others are discrete (which we sum over)”.
Identical particles

- Identical particles share all measurable physical characteristics: mass, charge, spin . . .

- In classical mechanics, the particles may be distinguished by attaching a label to each coordinate, i.e., $\vec{x}_k$. Since we can track each particle in time, we can say “at time $t$, particle $k$ was at $\vec{x}_k(t)$”.

- Problem: This contradicts quantum mechanics. There is no way to continuously measure the position of each particle in a quantum system.

- Consequence: In quantum physics, indistinguishability is a fundamental concept and profoundly alters the physical properties of a system.
Configuration space of identical particles

- For $N$ identical particles on a manifold $\mathbb{X}$, the configuration space is

$$\mathbb{X}^N / S_N$$  (also a manifold)

\[\textbf{Figure: }\] Illustration of identification of different permutations of points $x_1$, $x_2$ and $x_3$. In $\mathbb{X}^3$ (left), exchanging $x_i$ and $x_j$ leads to different points, while on $\mathbb{X}^3 / S_3$ these points are identified. The result is actually a manifold.
Hilbert space for identical particles

- Working with $L^2(\mathbb{X}^N/S_N)$ is cumbersome.
- But: If $\dim(\mathbb{X}) \geq 3$, the Hilbert space $L^2(\mathbb{X}^N/S_N)$ contains two components. Each is isomorphic to the symmetric and anti-symmetric part of $L^2(\mathbb{X}^N)$, respectively. Note: $L^2(\mathbb{X}^N) = L^2(\mathbb{X})^N$.
- $\Psi(x_1, \cdots, x_N)$ is called symmetric if for every $\sigma \in S_N$
  \[
P_\sigma \Psi(x_1, \cdots, x_N) := \Psi(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \Psi(x_1, \cdots, x_N).
\]
- $\Psi(x_1, \cdots, x_N)$ is called anti-symmetric if for every $\sigma \in S_N$
  \[
P_\sigma \Psi(x_1, \cdots, x_N) = \text{sgn}(\sigma)\Psi(x_1, \cdots, x_N).
\]
- The (anti-)symmetric functions in $L^2(\mathbb{X}^N)$ constitute a closed subspace, with projector $\Pi_+ (\Pi_-)$, and is thus a Hilbert space on its own.
Fermions and bosons

- It seems to be a fundamental law of nature, that particles fall into one of two categories:

  \[
  \begin{align*}
  \text{bosons:} & \quad P_{\sigma} \Psi = \Psi \\
  \text{fermions:} & \quad P_{\sigma} \Psi = \text{sgn}(\sigma)\Psi
  \end{align*}
  \]

- Thus, if we study fermions, we work with the anti-symmetric part of \( L^2(\mathbb{X}^N) \), while we use the symmetric part for bosons. (These have projectors \( \Pi_- \) and \( \Pi_+ \), respectively.)

- Typical fermions are electrons, protons, neutrons. Typical bosons are photons and composite particles (such as the hydrogen atom).

- From now on, we work with fermions.
We consider two fermions living on \((0, 1)\), with \(S = \{\uparrow, \downarrow\}\) being the discrete set:

- For one particle: \(\mathbb{X} = (0, 1) \times S\)
- For two particles: \(\mathbb{X}^2 = (0, 1)^2 \times S^2\)

Hilbert space:

\[ \mathcal{H} = \Pi - L^2(\mathbb{X} \times S^2). \]

The coordinate of particle \(k\) on the manifold \(\mathbb{X}\) is \(\xi_k := (x_k, s_k)\), so \(\Psi\) is a function of \(\xi_1\) and \(\xi_2\):

\[ \Psi = \Psi_{s_1, s_2}(x_1, x_2) \]

Antisymmetry:

\[ \Psi_{s_2, s_1}(x_2, x_1) = -\Psi_{s_1, s_2}(x_1, x_2). \]

Inner product:

\[ \langle \Psi | \Phi \rangle = \sum_{s_1, s_2} \langle \Psi_{s_1, s_2} | \Phi_{s_1, s_2} \rangle \quad \text{(inner prod. on } L^2(\mathbb{X})) \]
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Ok, breathe and relax . . .

Forget all about configuration space and discrete degrees of freedom. Now we’re gonna focus on the anti-symmetry thing and construct a basis for the $N$-body Hilbert space.

Our starting point now is the fact that:

1. We are given an ONB for $\mathcal{H}_1 = L^2(\mathbb{X})$ — i.e., one-particle Hilbert space
2. $L^2(\mathbb{X}^N) = L^2(\mathbb{X})^N$ (not obvious, but true for spaces of interest, at least)
3. $N$-fermion Hilbert space is $\mathcal{H}_N = \prod L^2(\mathbb{X}^N)$

Our goal: Obtain a basis for $\mathcal{H}_N$ for all $N$. This basis is the most important thing in many applications.
Slater determinants

- **Given** an orthonormal basis for $\mathcal{H}_1 = L^2(\mathbb{R})$:

  \[ \{ \phi_n : n = 1, 2, \ldots \} \]

- $\mathcal{H}_1^N$ has then an orthonormal basis

  \[ \{ \Phi_{n_1, \ldots, n_N} := \phi_{n_1} \otimes \cdots \otimes \phi_{n_N} \} \]

- For any $\Psi \in \mathcal{H}_N = \Pi_+ \mathcal{H}_1^N$, we have

  \[ \Psi = \sum_{\vec{n}} c_{n_1, \ldots, n_N} \Phi_{n_1, \ldots, n_N}. \]

- $\Psi \in \mathcal{H}_N$ is antisymmetric, so for any $\sigma \in S_N$:

  \[ P_\sigma \Psi = \sum_{\vec{n}} c_{\vec{n}} \Phi_{\sigma(\vec{n})} = \sum_{\vec{n}} c_{\sigma^{-1}(\vec{n})} \Phi_{\vec{n}} = \sum_{\vec{n}} \text{sgn}(\sigma) c_{\vec{n}} \Phi_{\vec{n}} \]

- Thus:

  \[ c_{\sigma(\vec{n})} = \text{sgn}(\sigma) c_{\vec{n}}, \quad \forall \sigma \in S_N \]
Slater determinants 2

- In particular: If $n_j = n_k$ for $j \neq k$, $c_{\vec{n}} = 0$.
- We note that we may write:

$$\Psi = \sum_{n_1 < n_2 < \ldots} \sum_{\sigma \in S_N} c_{\vec{n}} \text{sgn}(\sigma) \Phi_{\sigma(\vec{n})} =: \sum_{n_1 < n_2 < \ldots} \sqrt{N!} c_{\vec{n}} \Phi_{\vec{n}}^{SD}.$$  

- The Slater determinants can be written:

$$\Phi_{\vec{n}}^{SD} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{n_1}(x_1) & \cdots & \phi_{n_1}(x_N) \\ \vdots & \ddots & \vdots \\ \phi_{n_N}(x_1) & \cdots & \phi_{n_N}(x_N) \end{vmatrix}$$

- They are orthonormal (easy to show) and constitute a basis for $\mathcal{H}_N = \Pi_- \mathcal{H}_1^N$. Due to double (or $N!$) counting, we need $n_1 < n_2 < \ldots < n_N$.  

Pauli exclusion principle

We now have an interesting observation: The index $\vec{n}$ for the Slater determinant basis is replaced by a subset of $N$ integers, since permutations are identified. This is a statement of the indistinguishability of the particles! Particles are “disallowed to be in the same one-particle state $\phi_n$”.

Figure: The basis $\Phi_{\vec{n}}$ for $\mathcal{H}_1^N$ is enumerated by ordered sets of $N$ integers, while the basis for $\mathcal{H}_N$ is enumerated by unordered sets.
Creation and annihilation operators

From the fact:

\[ \mathcal{B}_N \text{ for } \mathcal{H}_N \longleftrightarrow \text{subsets of } N \text{ integers} \]

we may consider constructing \( \mathcal{B}_{N \pm 1} \) from \( \mathcal{B}_N \) by adding/removing an element to the set.

Moreover:

\[ \text{subsets of } N \text{ integers } \longleftrightarrow \text{int’s with } N \text{ nonzero binary digits} \]

Example:

\[ \vec{n} = \{3, 5, 8\} \longleftrightarrow \alpha = \cdots 00010010100b \]

So setting or clearing a bit nicely describes the basis mapping.
Creation and annihilation operators 2

- For $\alpha \in \mathbb{N}$, define $\#\alpha =$ number of nonzero bits in binary representation. We may regard $\alpha$ as a subset of integers, with unions, intersections, . . .
- We may write $\Phi_{\alpha}^{SD}$ or $\Phi_{n}^{SD}$ with no danger of confusion.
- By considering properties of determinants, we may construct $\mathcal{B}_{N+1}$ by adding a row/column to all the $N$-particle Slater determinants.
- This results in the definition of a creation operator $c_{n}^{\dagger}$ for each $n = 1, 2, \ldots$. This adds a row/column and reorders the determinant so that $n_1 < n_2 < \ldots$. Thus:

$$
c_{n}^{\dagger} \Phi_{\alpha}^{SD} = \begin{cases} (-1)^{j} \Phi_{\alpha \cup \{n\}}^{SD} & \text{if } n \notin \alpha \\ 0 & \text{if } n \in \alpha \end{cases}
$$

The sign change comes from the reordering needed to obtain a Slater determinant with ordered indices.
- By linear extension, $c_{n}^{\dagger}$ is a linear operator that maps $\mathcal{B}_{N}$ onto $\mathcal{B}_{N+1}$. 
Creation and annihilation operators 3

- For all \( n \), \( c_n^\dagger : \mathcal{H}_N \to \mathcal{H}_{N+1} \) is bounded with norm 1. (Obviously!)
- The adjoint \( c_n : \mathcal{H}_{N+1} \to \mathcal{H}_N \) is called an annihilation operator.
- The dagger notation is standard in physics, so we adopt it.
- Fact:

\[
\{c_n, c_m\} = 0, \quad \{c_n, c_m^\dagger\} = \delta_{n,m} 1, \quad \text{where} \quad \{A, B\} := AB + BA
\]

- By defining \( \mathcal{H}_0 \) as some (arbitrary) one-dimensional space with basis vector (“the vacuum”) \( \Phi_{SD}^0 \), we have:

\[
\Phi_{n_1, n_2, \ldots, n_N}^{SD} = c_{n_1}^\dagger c_{n_2}^\dagger \cdots c_{n_N}^\dagger \Phi_{SD}^0, \quad n_1 < n_2 < \cdots
\]

i.e., all Slater determinants can be generated from vacuum using creation operators.

- This is actually a quite vivid and natural description of the underlying mathematics.
Fock space

- For any $\Psi \in \mathcal{H}_N$:

$$\Psi = \sum_{\alpha, \# \alpha = N} c_{\alpha} \Phi_{\alpha}^{SD}.$$  

Or, equivalently:

$$\mathcal{H}_N = \bigoplus_{\alpha, \# \alpha = N} \text{Span}(\Phi_{\alpha}^{SD}) \quad \text{(closure implied)}.$$  

- Fock space can be defined as:

$$\tilde{\mathcal{H}} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N = \bigoplus_{\alpha} \text{Span}(\Phi_{\alpha}^{SD}),$$  

i.e., all Slater determinants with varying number of particles naturally define one big mother of a QM Hilbert space.
A hint at the usefulness

- Often, questions depend on the number of particles present, and we have seen that the Hilbert space has a very complicated structure for many particles.

- On the other hand, we have seen that from a basis for, e.g., $L^2(\mathbb{R}^3)$, or some approximation such as finite element spaces, the corresponding $N$-body space can “easily” be manipulated using creation and annihilation operators. Implementations can be done using clever bit-pattern manipulations already hinted at.

- Moreover, we shall see later that even the Hamiltonian has a simple form for arbitrary number of particles using $c_n^\dagger$ and $c_n$. 
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