# $\infty$-state problems and an application to the free particle

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# Outline

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# Basis functions for waves

Normalizable wave functions are in the Hilbert space of square integrable complex functions, sometimes called $\mathcal{L}^2$. A basis is given by the plane waves, although the plane waves themselves do not lie in $\mathcal{L}^2$. We resolve this problem first.

In (infinite) $D$-dimensional space, introduce the position operator $\hat{\mathbf{r}}$ and the momentum operator $\hat{\mathbf{p}}$. The eigenstates are $\hat{\mathbf{r}}\,|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle$ and $\hat{\mathbf{p}}\,|\mathbf{p}\rangle = \mathbf{p}\,|\mathbf{p}\rangle$. The normalized eigenstates are complete, and therefore each forms a basis—

$$\int d\mathbf{r}\ \ |\mathbf{r}\rangle\,\langle\mathbf{r}| = 1 \quad \text{and} \quad \int d\mathbf{p}\ \ |\mathbf{p}\rangle\,\langle\mathbf{p}| = 1.$$

The wavefunction of $|\psi\rangle$ is the function $\langle\mathbf{r}|\psi\rangle = \psi(\mathbf{r})$. This is an expansion of the state in the eigenbasis of $\hat{\mathbf{r}}$. The position and momentum eigenstates become

$$\langle\mathbf{r}|\mathbf{p}\rangle = \frac{1}{\sqrt{(2\pi)^D}}\mathrm{e}^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \quad \text{and} \quad \langle\mathbf{r}|\mathbf{r}'\rangle = \delta^D(\mathbf{r}-\mathbf{r}').$$

# Representations of operators

The two basic operators $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ must be infinite dimensional. Now we examine their matrix representations in the eigenbasis of $\hat{\mathbf{r}}$. First note

$$\langle \mathbf{r}|\,\hat{\mathbf{r}}\,|\psi\rangle = \int d\mathbf{x}\;\langle \mathbf{r}|\,\hat{\mathbf{r}}\,|\mathbf{x}\rangle\,\langle \mathbf{x}|\,\psi\rangle = \int d\mathbf{x}\;\mathbf{x}\delta^D(\mathbf{r}-\mathbf{x})\psi(\mathbf{x}) = \mathbf{r}\psi(\mathbf{r}).$$

So $\hat{\mathbf{r}}$ is diagonal and corresponds to multiplication by $\mathbf{r}$. The operator $\hat{\mathbf{r}}$ is clearly Hermitean. Is this obvious? Next:

$$\begin{aligned}\langle \mathbf{r}|\,\hat{\mathbf{p}}\,|\psi\rangle &= \int d\mathbf{p}d\mathbf{x}\;\langle \mathbf{r}|\,\hat{\mathbf{p}}\,|\mathbf{p}\rangle\,\langle \mathbf{p}|\mathbf{x}\rangle\langle \mathbf{x}|\psi\rangle = \int d\mathbf{p}d\mathbf{x}\;\mathbf{p}\mathrm{e}^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{x})/\hbar}\psi(\mathbf{x}) \\ &= \int d\mathbf{p}\;\mathbf{p}\mathrm{e}^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\widetilde{\psi}(\mathbf{p}) = -\int d\mathbf{p}\;i\hbar\frac{d}{d\mathbf{r}}\mathrm{e}^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\widetilde{\psi}(\mathbf{p}) \\ &= -i\hbar\frac{d}{d\mathbf{r}}\psi(\mathbf{r}).\end{aligned}$$

(Is $\hat{\mathbf{p}}$ Hermitean?)

# The basic commutator

We evaluate the commutator $[\hat{\mathbf{r}}, \hat{\mathbf{p}}]$ using the representations of the operators in the chosen basis. The commutator itself is an operator which acts on the space $\mathcal{L}^2$. So we take a square integrable function $f(\mathbf{r})$ and evaluate the commutator on this—

$$[\hat{r}_j, \hat{p}_k] f(\mathbf{r}) = i\hbar \left( \frac{d r_j f(\mathbf{r})}{d r_k} - r_j \frac{d f(\mathbf{r})}{d r_k} \right) = i\hbar \delta_{jk} f(\mathbf{r}).$$

The commutator is then $[\hat{r}_j, \hat{p}_k] = i\hbar\delta_{jk}$.

A straightforward induction can be used to show that

$$[\hat{r}_j, \hat{p}_k^n] = i\hbar\delta_{jk} n (\hat{p}_k)^{n-1}. \quad \text{therefore} \quad [\hat{r}_j, f(\hat{p}_k)] = i\hbar\delta_{jk} f'(\hat{p}_k).$$

The Baker-Campbell-Hausdorff relation is

$$\mathrm{e}^A \mathrm{e}^B = \exp\left[ A + B + \frac{1}{2}[A, B] + \cdots \right],$$

where the dots denote multiple commutators. This can be checked using the Taylor expansion of the exponential.

# Two problems

## Problem 6.1: Change of basis

States in the momentum basis are $\langle \mathbf{p}|\psi\rangle$.

1. How are they related to the wavefunction? What are the elements of the unitary matrix which makes this change of basis?
2. What are the new representations of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$?
3. Check that the commutator $[\hat{\mathbf{p}}, \hat{\mathbf{r}}]$ is independent of basis.

## Problem 6.2: The Baker-Campbell-Hausdorff formula

Find a method to generate any term of the Baker-Campbell-Hausdorff formula. Implement this in Mathematica, and examine the first 35 terms.

# Translation operators

Consider the operator $\hat{T}(\mathbf{x}) = \exp(-i\mathbf{x}\cdot\hat{\mathbf{p}}/\hbar)$. Since $\hat{\mathbf{p}}$ is Hermitean, $\hat{T}$ is unitary (for real $\mathbf{x}$). Also, since the $\hat{p}_j$ commute amongst themselves, the exponential factors into pieces $\hat{T}_j(x_j) = \exp(-ix_j\hat{p}_j/\hbar)$. It is easy to check that $\hat{T}_j^{-1}(x_j) = \exp(ix_j\hat{p}_j/\hbar)$, so that $\hat{T}^{-1}(\mathbf{x}) = \hat{T}(-\mathbf{x})$. Also,

$$[\hat{r}_j, \hat{T}(\mathbf{x})] = x_j\hat{T}(\mathbf{x}).$$

If $\hat{\mathbf{r}}\,|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle$, then it follows that $\hat{\mathbf{r}}\,\hat{T}(\mathbf{x})\,|\mathbf{r}\rangle = (\mathbf{r}+\mathbf{x})\,\hat{T}(\mathbf{x})\,|\mathbf{r}\rangle$. This implies that

1. $\hat{T}(\mathbf{x})\,|\mathbf{r}\rangle = |\mathbf{r}+\mathbf{x}\rangle$.
2. The eigenvalues of $\hat{\mathbf{r}}$ are continuous and infinite.
3. The Hilbert space is infinite dimensional.

## Generating translations

Take the infinitesimal translation operator

$$\hat{T}(\delta\mathbf{x}) \simeq 1 - \frac{i}{\hbar}\delta\mathbf{x}\cdot\hat{\mathbf{p}} = 1 + \delta\mathbf{x}\cdot\nabla.$$

Acting on any function $f(\mathbf{r})$, its action is

$$\hat{T}(\delta\mathbf{x})f(\mathbf{r}) \simeq [1 + \delta\mathbf{x}\cdot\nabla]\, f(\mathbf{r}) = f(\mathbf{r}+\delta\mathbf{x}).$$

So this translation operator generates infinitesimal translations, provided the derivative of the function exists.
Expanding the exponential to all orders, one sees that the translation operator generates exactly the full Taylor expansion of a test function—

$$\hat{T}(\delta\mathbf{x})f(\mathbf{r}) = \left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(\delta\mathbf{x}\cdot\nabla\right)^n\right] f(\mathbf{r}).$$

So every translation operator generates exactly the expected translation on sufficiently smooth test functions.

# Groups

A group consists of a set of elements $G = \{g_i\}$ and an operation of multiplication between them such that

1. If $g_i$ and $g_j$ are elements of $G$ then so is the product $g_i g_j$.
2. There exists an unique element called the identity such that $I g_i = g_i$.
3. For every element $g_i \in G$, there is an unique element $g_i^{-1} \in G$ such that $g_i g_i^{-1} = I$.
4. For $g_i$, $g_j$ and $g_k$ in $G$, $(g_i g_j) g_k = g_i (g_j g_k)$.

Example 1: The set $\{1, \sigma_1\}$ is a group under matrix multiplication. This is called the group $Z_2$, or the group of permutations of two objects. The elements of the group commute. Such groups are called Abelian groups.

Example 2: The set of all $2 \times 2$ unitary matrices is a group under matrix multiplication. This group is denoted U(2). The elements of this group do not commute. Since there is a continuous infinity of the elements, this is called a continuous group.

# The translation group

Consider the set of translation operators $\hat{T}(\mathbf{x})$ for all $\mathbf{x}$. The operation of multiplication is defined to be the result of successive translations. Then we find:

1. $\hat{T}(\mathbf{x})\hat{T}(\mathbf{y})\left|\mathbf{r}\right\rangle = \hat{T}(\mathbf{x})\left|\mathbf{r}+\mathbf{x}\right\rangle = \left|\mathbf{r}+\mathbf{y}+\mathbf{x}\right\rangle = \hat{T}(\mathbf{y}+\mathbf{x})\left|\mathbf{r}\right\rangle$. So the set is closed under multiplication.
2. $\hat{T}(\mathbf{0})$ is the identity.
3. For every translation by $\mathbf{x}$, the translation by $-\mathbf{x}$ is the inverse.
4. Multiplication is associative.

Since there is a continuous infinity of elements, the group of translations is a continuous group. It is also an Abelian group.

The translation group acting on the Hilbert space of position eigenstates is isomorphic to the group of vector additions in the Euclidean space $R^D$.

# Schrödinger's differential equation

The quantum evolution (Schrödinger's) equation is

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle .$$

In the special case of a single particle of mass $m$ in a central potential the classical Hamiltonian is $H = \mathbf{p}^2/(2m) + V(\mathbf{r})$. The corresponding quantum Hamiltonian is the operator $\hat{H} = \hat{\mathbf{p}}^2/(2m) + V(\hat{\mathbf{r}})$.

## Problem 6.3: Single particle evolution equation

By taking matrix elements of $\hat{H}$ in eigenstates of $\hat{\mathbf{r}}$, *i.e.*, by examining $\langle\mathbf{r}'|\hat{H}|\mathbf{r}\rangle$, show that one gets the usual differential equation

$$i\hbar\frac{d\psi(\mathbf{r})}{dt} = \hat{H}\psi(\mathbf{r}), \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}).$$

# Translationally symmetric Hamiltonian

Let us examine the Hamiltonians which have translation invariance. In these cases $[\hat{H}, \hat{T}(\mathbf{x})] = 0$. Recall that

$$[\hat{\mathbf{r}}, \hat{T}(\mathbf{x})] = \mathbf{x}\hat{T}(\mathbf{x}) \neq 0.$$

So $\hat{H}$ cannot involve $\hat{\mathbf{r}}$ if it is to be translation symmetric. This implies that $V(\hat{\mathbf{r}})$ is constant, and therefore the particle is moving without any force acting on it.

This is a proof that the only translational symmetric Hamiltonians are those for a free particle. Call this the Hamiltonian $\hat{H}_0$. We have proved that $\hat{H}_0 = \hat{\mathbf{p}}^2/(2m) = -(\hbar^2/2m)\nabla^2$.

Since $\hat{\mathbf{p}}$ and $\hat{H}_0$ commute, the solutions of this Schrödinger equation must be momentum eigenstates, *i.e.*, plane waves. We have already investigated these wavefunctions $\langle\mathbf{r}|\mathbf{p}\rangle$.

# Outline

# A free particle

The free particle Hamiltonian is

$$\hat{H}_0 = \frac{1}{2m}\hat{\mathbf{p}}^2,$$

and it describes a particle which is invariant under translations. Since $[\hat{H}_0, \hat{\mathbf{p}}] = 0$, these operators can be diagonalized simultaneously. Since the eigenstates of $\hat{\mathbf{p}}$ are non-degenerate (being the plane-wave states), $\hat{H}_0$ is diagonalized in this basis. However, the eigenvalues of $\hat{H}_0$ are doubly degenerate: $E_0 = \mathbf{p}^2/2m$, having equal values for $\pm\mathbf{p}$.

We have shown that all elements of the translation group commute with $\hat{H}_0$, so they are simultaneously diagonalizable. However, in the diagonal basis of the translation group, $\hat{H}_0$ still has degenerate eigenvalues. So there must be some other operator which commutes with $\hat{H}_0$. As a result, the symmetry group of the free particle must be larger than that of translations.

# Parity

The symmetry that we have missed out in the previous analysis is parity. First we consider its properties in classical mechanics. It is a $D \times D$ matrix acting on vectors: $\Pi\mathbf{r} = -\mathbf{r}$, $\Pi\mathbf{p} = -\mathbf{p}$. So, in the vector space $R^D$ it must have the representation $\Pi = -I$. The set $\{I, \Pi\}$ forms a group.

We are interested in the operator $\hat{\Pi}$ acting on the Hilbert space of quantum states of the free particle. Acting on momentum eigenstates it must have the representation $\hat{\Pi}\left|\mathbf{p}\right\rangle = \left|-\mathbf{p}\right\rangle$.

**Problem 6.4: Parity**

Evaluate the commutators $[\hat{\Pi}, \hat{\mathbf{p}}]$ and $[\hat{\Pi}, \hat{T}(\mathbf{x})]$. Prove that $[\hat{\Pi}, \hat{\mathbf{p}}^2] = 0$, so $[\hat{\Pi}, \hat{H}_0] = 0$. Prove that there are no other operators which commute with $\hat{H}_0$.

# Parity projections

Construct the projection operators $\hat{P}_\pm = (1 \pm \hat{\Pi})/2$. These are Hermitean since $\hat{\Pi}$ is Hermitean. Since $\hat{P}_+^2 = \hat{P}_+$ and $\hat{P}_-^2 = \hat{P}_-$, their eigenvalues are 1 or 0. Also $\hat{P}_+\hat{P}_- = \hat{P}_-\hat{P}_+ = 0$, and hence they project onto orthogonal subspaces.

Clearly $\hat{\Pi}\hat{P}_\pm = \pm\hat{P}_\pm$, so the states $\hat{P}_\pm |\psi\rangle$ are eigenstates of $\hat{\Pi}$.

Any state $|\psi\rangle$ can be split into a positive parity state $|\psi, +\rangle = \hat{P}_+ |\psi\rangle$ and a negative parity state $|\psi, -\rangle = \hat{P}_- |\psi\rangle$. Since $\hat{P}_+ + \hat{P}_- = 1$, there is no other component.

From the eigenstates of the free particle Hamiltonian, $|E_0\rangle$, one can construct $\hat{P}_\pm |E_0\rangle = |E_0, \pm\rangle$, such that

$$\langle \mathbf{r}|E_0, +\rangle = \frac{\cos(\mathbf{p}\cdot\mathbf{r}/\hbar)}{\sqrt{(2\pi)^D}} \quad \text{and} \quad \langle \mathbf{r}|E_0, -\rangle = \frac{\sin(\mathbf{p}\cdot\mathbf{r}/\hbar)}{\sqrt{(2\pi)^D}}$$

In this basis $\hat{H}_0$ and $\Pi$ are diagonal.

# Wave packets

The states $|E_0, \pm\rangle$ are not in $\mathcal{L}^2$. One can construct normalized wave functions in either of two ways. The older way is to make linear combinations of plane waves which are in $\mathcal{L}^2$, called wavepackets—

$$\psi(t, \mathbf{r}, \lambda) = \int d\mathbf{p} \widetilde{\psi}(\mathbf{p}, \lambda) \mathrm{e}^{-iEt/\hbar} \langle \mathbf{r} | \mathbf{p}, \lambda \rangle, \quad \text{where} \quad \lambda = \pm 1.$$

Wavepackets are not eigenstates of $H_0$. However, we have arranged for them to be eigenstates of the parity operator. This means that the packets generically have even number of maxima which approach each other (or recede from each other) in time.

**Problem 6.5: Wavepackets**

Construct the expectation value of the momentum operator in any wavepacket, and show that the average velocity is related to the group velocity of the packet.

# Particle in a box

The modern method is to restrict the wavefunctions to lie within a box, $|\mathbf{r}| \leq L$. By imposing periodic boundary conditions $\psi(\mathbf{r}) = \psi(\mathbf{0}) = 0$, one picks only a subset of all possible momenta. Fourier integral transforms are replaced by Fourier series and eigenstates of the Hamiltonian are in $\mathcal{L}^2$.

One finds expectation values of all operators in the problem for finite $L$, and takes the limits of these expectation values as $L \to \infty$. Since physics is only concerned with observables and not with wavefunctions, this procedure is perfectly well defined.

The translation symmetry of the Hamiltonian is broken to a discrete subgroup, and parity symmetry is retained. The eigenfunctions of the Hamiltonian are $|\mathbf{p}, \pm\rangle$ where $p_j = 2\pi n_j/(2L)$. The boundary conditions on the wavefunction has given quantization of the energies: $E = (\pi/L)\sqrt{\sum_{j=1}^{D} n_j^2}$.

# Regularization

- Both methods are meant to resolve the problem that the eigenstates of $\hat{H}_0$ are not in $\mathcal{L}^2$. Both break the symmetry of $\hat{H}_0$.
- Wavepackets break translational symmetry completely, but can be made symmetric (or antisymmetric) under parity.
- We have not picked a basis in the wavepackets. This is a non-trivial problem, and requires much mathematical development.
- The eigenstates of $\hat{H}_0$ in a box retain a larger part of the symmetry of the original problem.
- Expectation values of the momentum and position for each of the eigenvectors in a box vanishes.
- One can construct wavepackets in a box. This not necessary, but provides an easier method of studying wavepackets than the formal theory of analytic functions.

# Problem 6.6: a finite lattice

Keep only a lattice of points $\mathbf{r} = a\mathbf{N}$, where the elements of $\mathbf{N}$ are integers, and $a$ is the lattice spacing. Take each component of $\mathbf{N}$ to vary from 1 to L. Clearly $\hat{\mathbf{r}}$ becomes a finite dimensional square matrix.

1. Define the Fourier transformations carefully: find the allowed values of $\mathbf{p}$, and the amplitudes $\langle \mathbf{r} | \mathbf{r}' \rangle$, and $\langle \mathbf{r} | \mathbf{p} \rangle$.
2. Exhibit the matrix representations of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ explicitly in the eigenbasis of $\hat{\mathbf{r}}$.
3. Find the commutator $[\hat{\mathbf{r}}, \hat{\mathbf{p}}]$. Does this depend on the precise definition of the amplitude $\langle \mathbf{r} | \mathbf{p} \rangle$.
4. Is the Hilbert space separable? Does it change character when $a \to 0$?

## Problem 6.7: ladder operators

In the previous problem one can consider two "nearest neighbour" lattice points which have the same coordinates except in the direction $j$. If $\mathbf{N}$ has components $N_i$, then the nearest neighbour vector, $\mathbf{M}^{(j)}$ has components $N_i$ except when $i = j$; and then $M_j^{(j)} = N_j \pm 1$.

Can one combine $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ into ladder operators which connect the states $|\mathbf{N}\rangle$ and $\left|\mathbf{M}^{(j)}\right\rangle$? Can you write down the ladder operators as a square matrix and examine it?

What is the algebra of such matrices? What are the commutation relations? What are their characteristic equations?

# Outline

# Keywords and References

## Keywords

Wavefunction, Fourier transformations, Baker-Campbell-Hausdorff formula, group, Abelian group, continuous group, isomorphism, translation invariance, free particle Hamiltonian, parity, projection operators, wavepackets, lattice, quantization.

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