Infinite-state problems: the free particle

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Outline

Basis functions for waves

Normalizable wave functions are square integrable. The Hilbert space of such complex functions is sometimes called $\mathcal{L}^2$. We have seen that a basis is given by the plane waves, although the plane waves themselves do not lie in $\mathcal{L}^2$. We rephrase all this in more formal language.
In 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 bases are complete—

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

As a result, any function can be expanded in either of these bases.
The **wavefunction** corresponding to a state $|\psi\rangle$ is the complex 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 in this basis are

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

Representations of operators

Since

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

in this representation $\hat{\mathbf{r}}$ corresponds to multiplication by $\mathbf{r}$. (**Is this obvious?**) The operator $\hat{\mathbf{r}}$ is clearly Hermitean.
The representation of $\hat{\mathbf{p}}$ is

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

(**Is $\hat{\mathbf{p}}$ Hermitean?**)
All functions of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ can be constructed using these results.

A problem

A change of basis can be constructed by using the completeness relations—

$$\langle \mathbf{p}|\psi\rangle = \int d^D\mathbf{r}\, \langle \mathbf{p}|\mathbf{r}\rangle \langle \mathbf{r}|\psi\rangle.$$

1. How are states in this representation related to the wavefunction?
2. What is the representation of $\hat{\mathbf{r}}$ in this basis?
3. What is the representation of $\hat{\mathbf{p}}$ in this basis?
4. Check that the commutator $[\hat{\mathbf{p}}, \hat{\mathbf{r}}]$ is independent of basis.

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 $\mathcal{L}^2$. 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.

The translation operator

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.

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, $(g_i g_j) g_k = g_i (g_j g_k)$.

The set $\{1, \sigma_1\}$ is a group under matrix multiplication. The elements of the group commute. Such groups are called **Abelian groups**.
The set of all 2×2 unitary matrices is a group under matrix multiplication. The elements of this group do not commute.
The translation operators $\hat{T}(\mathbf{x})$ form a group. The group multiplication is the action on an eigenstate of $\hat{\mathbf{r}}$. Since there is a continuous infinity of elements, this is called a continuous group. It is an Abelian group.

The Schrödinger equation

The quantum evolution equation

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

when expressed in the eigenbasis of $\hat{\mathbf{r}}$ becomes the Schrödinger's equation—

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

Here the Hamiltonian has been written out in the same representation assuming that the potential is time independent, and the particle has mass m.

If the Hamiltonian is symmetric under translations, then $[\hat{H}, \hat{T}(\mathbf{x})] = 0$. Since $\hat{\mathbf{p}}$ commutes with translations but $\hat{\mathbf{r}}$ does not, this implies that $V(\mathbf{r})$ must vanish. Thus, the problem reduces to that for free particles. The solutions of the Schrödinger equation are then plane waves, since they are eigenstates of translations.

Outline

A free particle

The **free particle Hamiltonian** is

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{p}}^2 = -\frac{\hbar^2}{2m}\nabla^2,$$

and it embodies a system which is invariant under translations, as discussed above. Since $[\hat{H}, \hat{\mathbf{p}}] = 0$, these two operators can be diagonalized simultaneously. Since the eigenstates of $\hat{\mathbf{p}}$ are non-degenerate (being the plane-wave states), $\hat{H}$ is diagonalized in this basis. However, the eigenvalues of $\hat{H}$ are doubly degenerate: $E = \mathbf{p}^2/2m$, having the same value for $\pm\mathbf{p}$.

This "accidental" degeneracy argues for an extended symmetry of the Hamiltonian. The symmetry that we have missed out in the above analysis is **parity**. Parity transforms coordinates as $\Pi\mathbf{r} = -\mathbf{r}$. Clearly, it also transforms $\Pi\mathbf{p} = -\mathbf{p}$. Acting on momentum eigenstates it must have the representation $\Pi|\mathbf{p}\rangle = |-\mathbf{p}\rangle$. Note that $\Pi^2 = 1$ and hence the set $\{1, \Pi\}$ form a group. (**Prove that Π is Hermitean and unitary**)

Parity projections

Construct the operators

$$P_+ = \frac{1}{2}(1+\Pi) \quad \text{and} \quad P_- = \frac{1}{2}(1-\Pi).$$

$P_\pm$ are Hermitean since Π is Hermitean. They have the algebra $P_+^2 = P_+$ and $P_-^2 = P_-$ (thus the eigenvalues of these operators are 1 or 0). Such operators are called **projection operators**. (**A pure state density matrix is a projection operator**). One also finds that $P_+P_- = P_-P_+ = 0$, and hence these two project on to orthogonal subspaces.

Any state $|\psi\rangle$ can be split into a positive parity state $|\psi,+\rangle = P_+|\psi\rangle$ and a negative parity state $|\psi,-\rangle = P_-|\psi\rangle$. Since $P_+ + P_- = 1$, there is nothing else.

Given the action of Π on $\mathbf{p}$, one finds that $[\hat{H},\Pi] = 0$. For any momentum eigenstate $|\mathbf{p}\rangle$, one constructs $\langle\mathbf{r}|\mathbf{p},+\rangle = \cos(\mathbf{p}\cdot\mathbf{r})/\sqrt{(2\pi)^D}$ and $\langle\mathbf{r}|\mathbf{p},-\rangle = \sin(\mathbf{p}\cdot\mathbf{r})/\sqrt{(2\pi)^D}$. Thus, the operators $\hat{H}$, Π are completely diagonalized in the basis $|\mathbf{p},\pm\rangle$. We will use this basis from now on. Note that $\hat{\mathbf{p}}$ is no longer diagonal.

Wave packets

We have constructed solutions of the Schrödinger equation for free particles. However, these solutions are plane waves, and therefore not in $\mathcal{L}^2$. In order to construct properly normalized wave functions we can proceed in any one of two ways.
The first is to construct linear combinations of plane waves which are in $\mathcal{L}^2$. These are called **wavepackets**—

$$\psi(t, \mathbf{r}, \lambda) = \int d^D\mathbf{p}\widetilde{\psi}(\mathbf{p}, \lambda)\mathrm{e}^{-iEt/\hbar}\langle\mathbf{r}|\mathbf{p}, \lambda\rangle,$$

(where $\lambda = \pm 1$). Note that the wavepackets are no longer eigenstates of the Hamiltonian. 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.

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 second method is to restrict the wavefunctions to lie within a box, $|\mathbf{r}| \le L$. By imposing the conditions $\psi(\mathbf{r}) = 0$ and $\psi'(\mathbf{r}) = 0$ at the edges of the box, one picks only a subset of all possible momenta: one deals with Fourier series instead of Fourier integral transforms. However, the eigenstates of the Hamiltonian are square integrable.

One can find the expectation values of all operators in the problem for any finite value of L, and take 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.

Note that we have broken the translation symmetry of the Hamiltonian explicitly but we can still retain the parity symmetry. Thus the eigenfunctions of the Hamiltonian are $|\mathbf{p}, \pm\rangle$ where $p_j = 2\pi n_j/(2L)$. The imposition of the boundary conditions on the wavefunction at the boundaries of the box has given rise to **quantization** of the energies: $E = (\pi/L)\sqrt{\sum_{j=1}^{D} n_j^2}$.

Some points of note

- If one wants to construct wavepackets with a single maximum, then one is forced to construct a linear combination of the two parity states. Then it is easier to work in the momentum basis.
- Note that states need not have the symmetry of the Hamiltonian: wavepackets are neither translationally invariant, nor need to be states of good parity.
- The construction of eigenstates of the Hamiltonian in a box solves the problem that the basis states lie outside the Hilbert space being constructed.
- Note that the expectation values of the velocity and position for each of the eigenvectors in a box vanishes. One can still construct wavepackets, and such wavepackets will have finite velocity in general.
- Both methods of “regularization” of the problem break the translational symmetry of the problem.

Outline

References

1. The Principles of Quantum Mechanics, by P. A. M. Dirac. The developments in this lecture are discussed in detail in this classic monograph by one of the founders of the subject.
2. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture are scattered through chapters 2 and 3 of this book. Several of the problems are instructive
3. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 2 of this book discusses, among other things, the representations discussed in this lecture.
4. Mathematical Methods for Physicists, by G. Arfken. This book contains chapters on matrices and Fourier transforms which will be useful throughout this course.