



THE SCHRÖDINGER EQUATION

Quantum Physics

THE SCHRÖDINGER EQUATION

by
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Title: **The Schrödinger Equation**

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Input Skills:

1. Define: free particle, harmonic function, phase factor, lifetime.
2. Solve second order differential equations and differentiate.
3. Unknown: assume (MISN-0-383).

Output Skills (Knowledge):

- K1. Define: eigenfunction, eigenvalue, stationary state, operator, linear operator, commutator or commutator bracket, expectation value.
- K2. Write the S-equation for a particle in both 1 and 3 dimensions, with or without a potential present, and write the wave function Ψ which solves the free-particle equations.
- K3. Write an expression for the probability density in 3 dimensions, given a normalized wave function Ψ .

Output Skills (Rule Application):

- R1. Calculate the expectation values of operators in both the coordinate and momentum representations.
- R2. Calculate the commutators of the operators listed in table 4-2 in both coordinate and momentum space representations.

Output Skills (Problem Solving):

- S1. Derive the time-independent Schrodinger equation (4.54) by the technique of separation of variables, and write the time-dependent wave function $\Psi(r, t)$ in terms of the time-independent wave function and the energy E .
- S2. Show that the expectation value of the Hamiltonian in a stationary state is constant in time and equal to the energy eigenvalue.

External Resources (Required):

1. E. E. Anderson, *Modern Physics and Quantum Mechanics*, W. B. Saunders (1971).

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1. Introduction

In previous units, we introduced the wave function Ψ . Since Ψ contains all the information about the location of a particle in space and time, its calculation from the dynamics (interactions or forces present) is the most fundamental problem in quantum mechanics. We attack this problem through the Schrodinger equation, a differential equation for Ψ which we introduce in this unit.

We shall also introduce the notion of *linear operators*. In quantum mechanics, each observable is represented by such an operator; and the possible results of a measurement are directly related to the outcome of operations with the appropriate operator.

Since the material we shall cover in this unit is crucial for our later work, the student should study this unit with special care.

2. Procedures

1. Read section 4.9. The free particle equations referred to are equations (4.39) and (4.41); they are special cases of equation (4.42) and its 1-dimensional cousin. Note that V in general is a function of position and so depends on x or \vec{r} .

This is our first contact with the most important operator in the world, the Hamiltonian \mathcal{H} . (An *operator* changes one wave- function into another, or, more generally, one *state* into another. The wavefunction Ψ is the *coordinate representation* of the *state* of the particle. The momentum space wavefunction, ϕ , is the *momentum space representation* of the *state*. The *state* exists independently of the particular representation used to describe it.) Note that \mathcal{H} *determines the time-development* of the wavefunction through the Schrodinger equation (S-equation).

2. The solutions are equations (4.36) and (4.40).
3. Equation (4.44) of section 4.10 is the required probability density. The rest of section 4.10 is optional; it essentially shows that it is consistent

with the S-equation to treat $|\Psi|^2$ as a probability density.

4. Read section 4.11 to obtain the definitions needed. Note that the same operator has different forms in different representations. However the physical quantities of interest are the *matrix elements* of the operators which are independent of the representation chosen. The *matrix element* of an operator A between two states a and b is defined by

$$\begin{aligned} \langle a|A|b \rangle &\equiv \int \Psi_a^*(\vec{r}, t) (A\Psi_b(\vec{r}, t)) d\tau \\ &= \int \phi_a(\vec{p}, t) (A\phi_b(\vec{p}, t)) dp_x dp_y dp_z, \end{aligned}$$

where $\Psi_{a,b}(\psi_{a,b})$ are the coordinate (momentum) space representations of the states a and b .

Exercise: Verify the second equality for the momentum and position operators.

5. Study and memorize table 4-2 *except or the last line which is incorrect*. The energy operator is the Hamiltonian \mathcal{H} , whose coordinate representation, $-\hbar^2\nabla^2/2m + V(\vec{r})$ you have already seen. What should its momentum representation be? The S-equation connects \mathcal{H} with the time-derivative, but the energy operator is \mathcal{H} .
6. Solve problem 4-21 to gain practice in calculating expectation values. *Note the definition* of the uncertainty in an operator, $\Delta A \equiv \sqrt{\langle (A - \langle A \rangle)^2 \rangle}$, introduced in equation (4.51). This is the more rigorous definition of uncertainty alluded to in Unit 3.
7. Solve problem 4-22 to gain practice in calculating commutators and an understanding of the fact the operators in general do not commute—**THE ORDER IN WHICH YOU APPLY THEM IS IMPORTANT!**
The question at the end of the problem is very important; and its answer shows that operators have an *algebra* (properties under multiplication) which is independent of the representation chosen.
8. Read section 4-12 through the end of the paragraph directly below equation (4.55). Study the steps leading to equations (4.54) and (4.55) and make sure you can reproduce them.

9. Read the rest of page 151 and continue through the end of the example on page 152. In general, an eigenvalue need not be real as indicated in the text. However, eigenvalues of operators corresponding to observables are always real, since they represent possible results of a measurement.
10. Read the remainder of section 4-12. You may omit the proof of the eigenvalues of \mathcal{H} , i. e. the possible energies of the system, are real. In the proof at the top of page 153, the first step should be

$$\langle E \rangle = \int \Psi^*(\vec{r}, t) (\mathcal{H}\Psi(\vec{r}, t)) d\tau.$$

The next step follows from the S-equation.

This proof fulfills Output Skill S2. As an exercise, prove the following more general statement:

Let $\Psi_E(\vec{r}, t)$ be a stationary state of energy E . Let Q be an operator such that $Q\Psi_E(\vec{r}, 0) = q\Psi_E(\vec{r}, 0)$; i. e. $\Psi_E(\vec{r}, 0)$ is an eigenfunction of Q with eigenvalue q . Then $\Psi_E(\vec{r}, t)$ is an eigenfunction of Q with eigenvalue q for all t . Moreover, the expectation value of Q for the state represented by Ψ_E is constant in time and equal to q .

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