APPLIED QUANTUM MECHANICS

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Preface

This book is based on the lectures given by Professor R. K. Osborn in two consecutive graduate courses on the applications of quantum mechanics to problems encountered in nuclear engineering. The manuscript, mostly in his handwriting, had been completed and submitted to the publisher shortly before the author suddenly passed away in February 1987. We, his students and colleagues, decided to go ahead with the publication of the book on his behalf.

During the editing process, we have interfered with the content and style of the manuscript as little as possible. Professor Osborn's approach to teaching quantum mechanics to nuclear engineering students represents a novel point of view in that it introduces the necessary concepts and tools of quantum mechanics using the density matrix formalism, and illustrates their utility by considering only those problems that are relevant to nuclear engineering (in a broad sense). In this respect, this book is very different from, and complimentary to, the existing text books on quantum mechanics, both in approach and content.

We dedicate our efforts in the publication of this book to the memory of this great teacher.

1988

A. Ziya Akcasu
Juan Carlos Lopez
George C. Summerfield
Sidney Yip

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Chapter 1

Introduction

The primary purpose of this book is to examine in an introductory, but quantitative way, some of the details of neutron-nuclear reactions. A necessary subsidiary to this purpose is some study of nuclear structure per se. And, since the subject at hand dwells in the realm of the microscopic rather than the macroscopic, it will be necessary to view it from the perspective of quantum mechanics rather than classical mechanics.

This point needs emphasis — the distinction between classical and quantum mechanics is merely one of perspective. Whatever the real world is all about, it has not changed in the past hundred years. But the techniques for observation and measurement have been enormously refined and enlarged, requiring a corresponding refinement and enlargement of our perspective on natural phenomena to facilitate interpretation and understanding. No doubt, further refinement and enlargement will be called for in the future.

The modification of perspective from classical to quantum, which was largely initiated and completed in the first quarter of this century, was sparked by a number of failures of the classical viewpoint. First of all, spectral analysis of the radiation from black bodies became precise enough that clear discrepancies between observation and classical theory were apparent. Planck resolved the matter (crudely speaking) by assuming that the energy states of the radiation field were discretely distributed, rather than continuously. Then significant differences appeared between theory and observation of specific heats of solids at low temperatures. So Einstein borrowed Planck's idea and assumed discretely distributed oscillator energy states for the atoms in the solid with consequent marked improvement in agreement between theory and measurement. At the same time, the dis-

creteness of the radiation emitted by atoms was giving classical theory fits. So Bohr borrowed from Planck and Einstein, added a few refinements of his own, and came up with the idea of discretely distributed energy states for the electrons in atoms. What was emerging was a clear call for a new perspective — one that recognizes the possibility, if not probability, that the states accessible to real systems are discretely, not continuously, distributed. Since the rules, axioms, or whatever extant at the time could not encompass this new awareness; new rules had to be invented — to include the old ones when applicable but to open up the possibility of interpreting the seemingly fundamental discreteness of natural phenomena when necessary. These new rules for guiding perspective constitute what has come to be called the quantum mechanics.

In an attempt to clarify this matter somewhat, let us consider the classical view of the motion of a point particle of mass, m, moving in a central force field describable by a potential, $V(r)$.

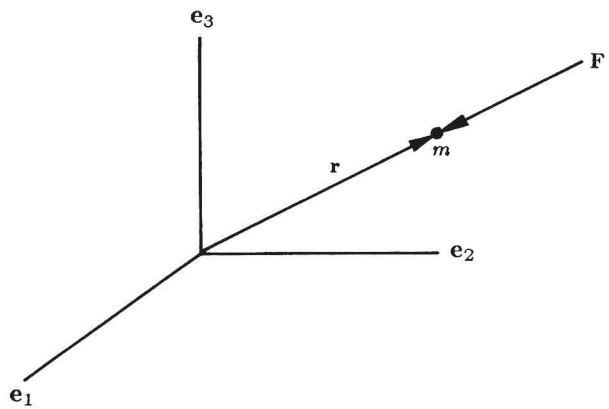

Fig. 1.1.

The rules employed in this situation are usually borrowed from Newton, and read

$$\begin{aligned} \frac{d}{dt}\mathbf{P} &= \mathbf{F} = -\nabla V\,, \\ \mathbf{P} &= m\mathbf{v}\,, \\ \mathbf{v} &= \frac{d}{dt}\mathbf{r}\,. \end{aligned} \tag{1.1}$$

If V is a function of the magnitude of $\mathbf{r}$ only, then

$$\mathbf{F} = -\nabla V = -\hat{\mathbf{r}}\frac{\partial V}{\partial r}\,, \tag{1.2}$$

so that, for an attractive force, $\partial V/\partial r$ must be positive. In this instance we observe that the total energy of the particle is a constant of the motion, i.e.:

$$\frac{dH}{dt} = 0\,,$$

where

$$H = \frac{1}{2}mv^2 + V\,. \tag{1.3}$$

That the angular momentum is another constant of the motion is also easily established, i.e.,

$$\begin{aligned} &\frac{d}{dt}\mathbf{L} = \mathbf{r}\times\mathbf{F} = 0\,, \quad \text{where} \\ &\mathbf{L} = \mathbf{r}\times m\mathbf{v}\,. \end{aligned} \tag{1.4}$$

Since

$$\begin{aligned} L^2 &= (\mathbf{r}\times\mathbf{P})\cdot(\mathbf{r}\times\mathbf{P}) \\ &= r^2P^2 - (\mathbf{r}\cdot\mathbf{P})^2\,, \end{aligned} \tag{1.5}$$

we may display the total energy (recall Eq. (1.3)) as

$$H = \frac{(\hat{\mathbf{r}}\cdot\mathbf{P})^2}{2m} + \frac{L^2}{2mr^2} + V(r)\,. \tag{1.6}$$

To proceed further, and for the sake of explicitness, let us assume that $V = -Ze^2/r$ and note that $\hat{\mathbf{r}}\cdot\mathbf{P} = m\dot{r}$ and display

$$H = \frac{1}{2}m\dot{r}^2 + \frac{L^2}{2mr^2} - \frac{Ze^2}{r}\,. \tag{1.7}$$

The turning points of the orbits are the values of r satisfying Eq. (1.7) when $\dot{r} = 0$.

Now the crux of the matter is that, according to these arguments, there is a continuum of elliptic orbits and a continuum of hyperbolic orbits. But numerous observations on systems of this kind (hydrogen-like atoms) have clearly demonstrated that, at least, the bound (elliptic) orbits (states) are discretely distributed. Thus we must modify our perspective of this situation in order to accommodate these observations. Experience has revealed that the modifications required are probably at least as subtle and extensive as those discussed below and numerously applied throughout the remainder of these lectures.

In order to facilitate the introduction and delineation of the requisite change in viewpoint, it is convenient to contemplate for a moment the notion of a measurement. A measurement often consists of a recording

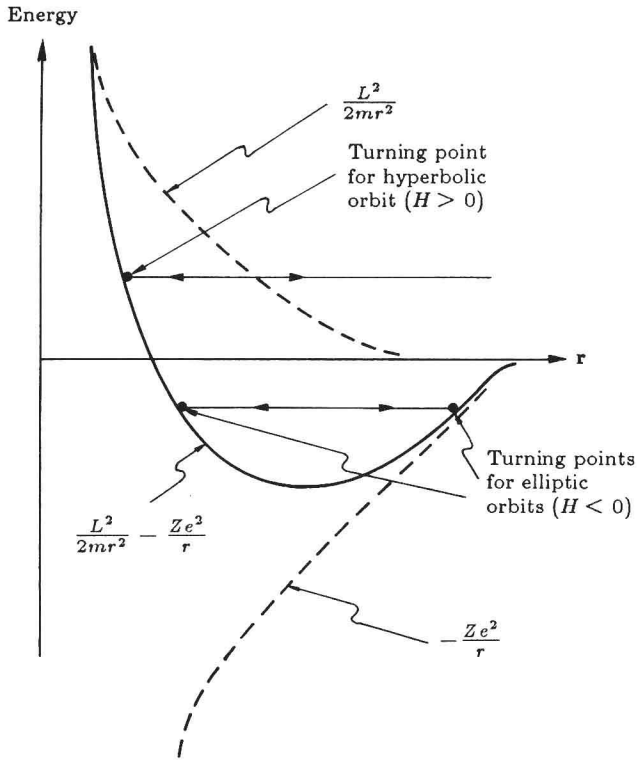

Fig. 1.2

of many numbers, each purportedly a quantitative realization of the same thing. Different observations often yield numbers of different magnitude, so an average of the results is usually performed to obtain a statistically significant estimate of the quantity to be measured. In other words, a measurement often consists of an experimental determination of an expectation value for the quantity of interest.

For example, suppose that Ω represents a quantity to be measured. Apparatus would then be devised to provide a number of realizations of Ω, say $\Omega_1, \Omega_2, \ldots, \Omega_j, \ldots, \Omega_N$, where N is the number of realizations for this particular measurement. Since the number of significant figures available by our apparatus is finite, if N is sufficiently large we find that many realizations are the same. That is, Ω_j may occur n_j times, and the ratio, n_j/N, is an experimental estimate of the probability of realizing Ω_j in a given try. Call this probability $P_{\text{meas}}(\Omega_j)$ i.e.,

$$P_{\text{meas}}(\Omega_j) = n_j/N\,. \tag{1.8}$$

The experimental estimate of an expectation value for the quantity to be measured is thus

$$\omega = \sum_j \Omega_j P_{\text{meas}}(\Omega_j) , \tag{1.9}$$

where the sum runs over those values of j for which the Ω_j are all different. We note in passing that the variance of this measurement is

$$V_{\text{meas}} = \sum_j \Omega_j^2 P_{\text{meas}}(\Omega_j) - \omega^2 . \tag{1.10}$$

Whatever rules of mechanics we accept, they must be adequate to guide us in interpreting measurements of this kind — as well as perhaps some others. Thus the rules must tell us how to compute the possible realizations of an observation — the Ω_j's, and also how to compute the probabilities of realizing a given value of Ω_j in a single try — the $P(\Omega_j)$'s. Furthermore, in order to understand how systems evolve in time it will also be necessary for the rules to tell us how to compute the probabilities that the system will undergo transitions from one state to another. As we have seen, the classical rules usually led us to the conclusion that the possible results of observations are continuously distributed — a conclusion contradicted by many studies, especially of microscopic systems.

The modern rules, which so far appear to fulfill all of these requirements quite successfully, and at the same time encompasses all of the old rules, will be introduced now and subsequently in bits and pieces; and extensively applied to a study of nuclear structure and neutron-nuclear reactions. To understand the measurement described above, we require first of all an operator, Ω_{op}, to represent the quantity to be measured — Ω. The eigenvalues of Ω_{op} will then represent the realizations of single observations (the Ω_j's) and hence must be real. (Do not be distressed if a certain amount of unfamiliar terminology crops up from time to time. Such matters will be clarified by examination and illustration subsequently.) It is assumed that the eigenfunctions, $|j\rangle$, of Ω_{op}, which satisfy the equations

$$\Omega_{\text{op}}|j\rangle = \Omega_j|j\rangle , \tag{1.11}$$

form a complete set.

Next we require a rule for the computation of the probabilities of realizing a given Ω_j in a single try. At the present time the rule states that these probabilities are given by the diagonal "matrix elements" of a probability operator, D, i.e.,

$$P_{\text{theor}}(\Omega_j) = \langle j|D|j\rangle . \tag{1.12}$$

By axiom, this probability operator is to be computed according to the Liouville equation, i.e.,

$$\begin{aligned}\frac{\partial D}{\partial t} &= \frac{i}{\hbar}(DH - HD) \\ &\equiv \frac{i}{\hbar}[D, H] \ ,\end{aligned} \tag{1.13}$$

where H is the system Hamiltonian (or energy operator — recall Eq. (1.6) for a particle in a central force field). Finally, the theoretical expectation value of Ω, to be compared with the measured one displayed in Eq. (1.9), is to be computed according to

$$\begin{aligned}\omega &= \sum_j \Omega_j P_{\text{theor}}(\Omega_j) \\ &= \sum_j \langle j|\Omega_{\text{op}}|j\rangle\langle j|D|j\rangle \\ &= \sum_j \Big(\sum_{j'} \langle j|\Omega_{\text{op}}|j'\rangle\langle j'|D|j\rangle\Big) \\ &= \text{Tr}\,\Omega_{\text{op}} D \ ,\end{aligned} \tag{1.14}$$

since the representation, $\{|j\rangle\}$, diagonalizes the operator, Ω_{op}. The notation, $\text{Tr}\,\Omega_{\text{op}} D$, means to take the trace (sum of diagonal elements) of the matrix product of the matrix elements of Ω_{op} and D.

This is about all of the rules we are going to need. The remainder of our task will be to clarify them somewhat, and implement them for application to specific cases. Initially, we concentrate on rule one — on the construction of operator representatives for observables and then the determination of their eigenfunctions and corresponding eigenvalues (possible results of observations). However, to assist us in this task we first note that, according to Eqs. (1.14) and (1.13),

$$\begin{aligned}\frac{\partial \omega}{\partial t} &= \text{Tr}\,\Omega_{\text{op}} \frac{\partial D}{\partial t} \\ &= \frac{i}{\hbar}\text{Tr}\,\Omega_{\text{op}}(DH - HD) \\ &= \frac{i}{\hbar}(\text{Tr}\,H\Omega_{\text{op}} D - \text{Tr}\,\Omega_{\text{op}} HD) \\ &= \frac{i}{\hbar}\text{Tr}(H\Omega_{\text{op}} - \Omega_{\text{op}} H)D \\ &= \frac{i}{\hbar}\text{Tr}[H, \Omega_{\text{op}}]D \ ,\end{aligned} \tag{1.15}$$

where we have assumed that $\Omega_{\rm op}$ itself is not explicitly time-dependent.

Purely for the sake of illustration, let us consider the problem of constructing operator representatives for the position, momentum, and energy of the previously discussed particle moving under the influence of a central force. At the outset we must note that this matter of identifying appropriate operator representatives of observables need not be accomplishable in a unique way. Furthermore, it is precisely with respect to these matters that we must proceed by a considerable exercise of ingenuity and guess work. For example, we might first guess that we can (in this instance) be guided by classical arguments in identifying the energy operator, i.e.,

$$H = \frac{P^2}{2m} + V \ . \tag{1.16}$$

So far so good, but what do we mean by the operators $\mathbf{P}$ and V (or $\mathbf{r}$, the position operator)? That is, what are the operands of $\mathbf{P}$ and $\mathbf{r}$, and what is the manner in which $\mathbf{P}$ and $\mathbf{r}$ operate upon their respective operands?

To illustrate terminology a little, consider a few common (and familiar) examples of operators and operands.

(a) Multiplication (the multiplication of f by g to produce h):

$$\underset{\text{operator}}{g}\underset{\text{operand}}{f} \longrightarrow h$$

(b) Differentiation:

$$\underbrace{\frac{d}{dx}}_{\text{operator}}\underbrace{f(x)}_{\text{operand}} \equiv \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \longrightarrow h(x)$$

(c) Integration:

$$\underbrace{\int_0^y dx}_{\text{operator}}\ \underbrace{f(x)}_{\text{operand}} \longrightarrow h(y)$$

(d) Matrix:

$$\underbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}_{\text{operator}} \underbrace{\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}}_{\text{operand}} \equiv \begin{pmatrix} af_1 + bf_2 \\ cf_1 + df_2 \end{pmatrix} \longrightarrow \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \ .$$

Note that all of these operators are linear. That is, if A is one of the operators, f and g are operands, and α and β are numbers, then

$$A(\alpha f + \beta g) = \alpha A f + \beta A g \ . \tag{1.17}$$

However not all of these operators commute with each other. That is, if A and B are two operators and if f is an operand for each, then

$$[A, B]f \equiv (AB - BA)f \neq 0$$

generally. For example

(a) Multiplicative operators commute by definition.

(b) Differentiation:

$$\frac{\partial}{\partial x}\frac{\partial}{\partial y}f(x,y) = \frac{\partial}{\partial y}\frac{\partial}{\partial x}f(x,y)$$

usually, so that

$$\left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right] f = 0 .$$

But

$$\frac{\partial}{\partial x}xf(x) \neq x\frac{\partial}{\partial x}f(x) ,$$

hence

$$\left[x, \frac{\partial}{\partial x}\right] f \neq 0 .$$

Actually

$$\left[x, \frac{\partial}{\partial x}\right] f = -f .$$

(c) Matrices: If A and B are two matrices, then

$$AB - BA = [A, B] = 0$$

only in very special cases.

We return now to the task of identifying operator representatives for momentum, $\mathbf{P}$, and position, $\mathbf{r}$, (or functions of position $V(r)$). As a first guess, let us assume that $\mathbf{r}$ is a multiplicative operator — so also is any function of $\mathbf{r}$. But what about $\mathbf{P}$? Consider the expected value (a measurable quantity) of $\mathbf{r}$, i.e.,

$$\langle \mathbf{r} \rangle = \mathrm{Tr}\, \mathbf{r} D . \tag{1.18}$$

By this we mean, as usual, that if $\{\psi_m\}$ is an appropriate, complete set of functions, then

$$\langle m|\mathbf{r}|n\rangle \equiv \int d\tau \psi_m^* \mathbf{r} \psi_n \qquad \text{and}$$

$$\langle m|D|n\rangle \equiv \int d\tau \psi_m^* D \psi_n \tag{1.19}$$

are square arrays of numbers, and

$$\begin{aligned}\langle \mathbf{r} \rangle &= \mathrm{Tr}\, \mathbf{r} D \\ &\equiv \sum_m \left(\sum_n \langle m|\mathbf{r}|n\rangle \langle n|D|m\rangle \right) . \end{aligned} \tag{1.20}$$

Now, as indicated by Eq. (1.15), we have

$$\frac{\partial}{\partial t}\langle \mathbf{r} \rangle = \frac{i}{\hbar}\mathrm{Tr}[H, \mathbf{r}]D \tag{1.21}$$

which, according to Eq. (1.16), becomes

$$\begin{aligned}\frac{\partial}{\partial t}\langle \mathbf{r} \rangle &= \frac{i}{\hbar}\mathrm{Tr}\left[\frac{P^2}{2m} + V, \mathbf{r}\right] D \\ &= \frac{i}{\hbar}\left[\mathrm{Tr}\left[\frac{P^2}{2m}, \mathbf{r}\right] D + \mathrm{Tr}[V, \mathbf{r}]D\right] . \end{aligned} \tag{1.22}$$

We have agreed to treat $\mathbf{r}$ (and hence $V(r)$ also) as a multiplicative operator, thus

$$[V, \mathbf{r}] = 0 \tag{1.23}$$

and

$$\frac{\partial}{\partial t}\langle \mathbf{r} \rangle = \frac{i}{\hbar}\mathrm{Tr}\left[\frac{P^2}{2m}, \mathbf{r}\right] D . \tag{1.24}$$

The mass of the particle, m, is just a number; and consequently to be regarded as a multiplicative operator. It is easily shown that, for any two operators A and B,

$$[A^2, B] = A[A, B] + [A, B]A . \tag{1.25}$$

Hence, Eq. (1.24) reads

$$\frac{\partial}{\partial t}\langle \mathbf{r} \rangle = \mathrm{Tr}\frac{i}{2m\hbar}\{P_j[P_j, \mathbf{r}] + [P_j, \mathbf{r}]P_j\}D . \tag{1.26}$$

Clearly $\mathbf{P}$ has to be identified as an operator that does not commute with $\partial\langle \mathbf{r} \rangle/\partial t \equiv 0$ which is most unreasonable. Instead, guided again by experience, we would like (or expect)

$$\begin{aligned}\frac{\partial}{\partial t}\langle \mathbf{r} \rangle &= \langle \mathbf{v} \rangle \\ &= \frac{1}{m}\langle \mathbf{P} \rangle . \end{aligned} \tag{1.27}$$