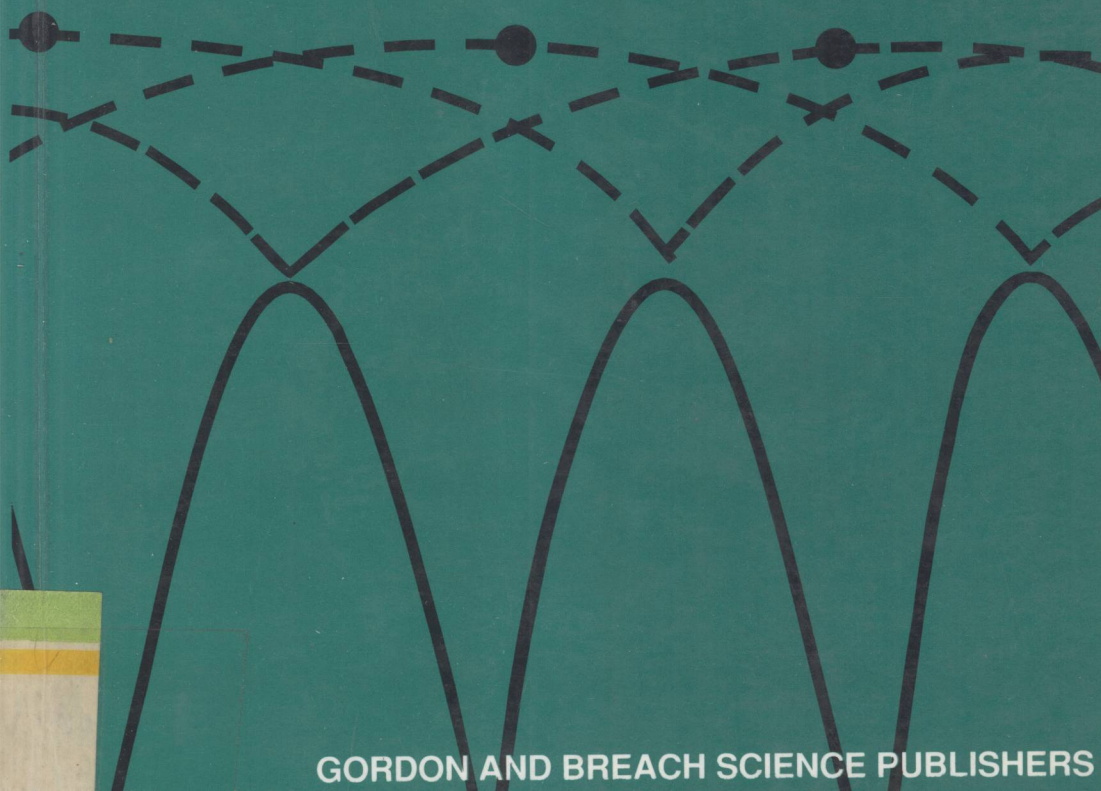
Introduction to the quantum theory of semiconductors

Marvin M. Cohen



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Introduction to the Quantum Theory of Semiconductors

For

my parents *Albert and Rose* who taught the value of learning

my wife *Anne* who lives the values of constancy

and

Vera Levy, who has always been by my side

Preface

This book grew out of the notes which I used to teach a short course in semiconductor theory at the American University, Washington, DC. The classes were made up of first-year graduate students in physics and engineering, many of whom were already working in semiconductor-related fields they had entered so-to-speak by the "back door," i.e. none had a formal background in semiconductors. It was our intention to develop a course in which these students and those planning to enter the field of semiconductors would get a mathematically oriented introduction to the methods, tools, and concepts which are fundamental to the theory of solids in general, with emphasis on applications to semiconductors.

The manuscript is aimed at students who have had an undergraduate modern physics course and an introductory course in thermodynamics. Chapters 1 and 2 are intended to serve as a review and not as a complete introduction. I have utilized many of the arguments and figures from a variety of sources and in many instances have modified the figure-labeling to correspond to presently accepted values and notation.

I would like to thank Herbert D. Curchack for much encouragement, Drs. Fernand Bedard, Charles Davis, Clyde Morrison, and Lynwood P. Randolph, and students Daniel J. Lanigan and James D. Penar for editing portions of the manuscript.

Preface to the Softcover Version

This softcover version of *Introduction to the Quantum Theory of Semiconductors* comes twenty-six years after the book made its debut in 1972. During the intervening quarter century, we have seen an unprecedented worldwide growth of information technology, primarily based on the unique physics of semiconductors. As I sit at one of my three home computers writing this new preface, I look back at the field when the hardcover version was printed; the desktop computer was not yet developed, semiconductor lasers were in their infancy, and the power of these materials to accelerate the rate of change of all technologies, and provide a worldwide information link that would influence world politics, was not yet dreamed of.

The book was written to cover in detail the many basic classical processes and the few known non-classical processes that enable all semiconductor devices to operate. For this reason, a quarter century later, it retains its unique ability to instruct students just entering the field as well as seasoned semiconductor engineers looking for new solutions.

Within the next ten years, the speed of computer chips will come up against a limit defined primarily by the velocity of an electron, and faster computers will be possible only through the development of new processes not subject to classical limits. I encourage students and engineers alike to work toward the development of such non-classical processes. In fact, one of these enabling processes has already been seminally developed—the ability of a particle to tunnel through an energy barrier in imaginary time. I believe that the next revolution in semiconductor technology will come as a result of the exploitation of such non-classical processes.

Contents

CHAPTER 1

Review of Quantum Theory

1.1 THE STATE OF A QUANTUM MECHANICAL SYSTEM

UNDERSTANDING of a subject or technology can be achieved only after an expenditure of effort to learn the language by which it may most conveniently be discussed. Because solid state physics is to a large measure based on the quantum theory, the theory of solids may be discussed by utilizing any of the quantum mechanical *representations*. For the student to work effectively in the field of solids, he must have a working knowledge not only of the wave-mechanical Schrödinger representation, but of all of the methods by which solids may be described. For this reason we shall start with a review of the abstract quantum theory as proposed by Dirac[1] from which all representations may be derived.

We shall assume that there exists a hypothetical many-dimensional space each point of which fully describes the state of our quantum mechanical system at time t. The state is assumed to be fully described by the coordinates of the particular point in the space or equivalently by a vector generated from the origin to the point. The many-dimensional vector that describes our state is called a *ket* vector and is written as $|A\rangle$. Thus $|A\rangle$ represents the state A of a quantum mechanical system. For example, as shown in Figure 1.1, the three dimensional velocity vector

$$|\mathbf{V}_{(t)}\rangle = a_{(t)}\,|\hat{V}_x\rangle + b_{(t)}\,|\hat{V}_y\rangle + c_{(t)}\,|\hat{V}_z\rangle \tag{1.1.1}$$

where $|\hat{V}_x\rangle$, $|\hat{V}_y\rangle$, and $|\hat{V}_z\rangle$ are the orthogonal unit velocity vectors (or basic vectors) which define our allowed velocity space, completely defines the state of the velocity of a system at any time t.

The Dual Space

In our study of semiconductor physics we shall make frequent use of the fact that for every vector space a unique dual space may be defined. We shall call the vectors in our dual space *bra* vectors and write them as $\langle B|$. We shall assume that for every ket vector $c|A\rangle$ in our original space there corresponds a bra vector $\langle A|c^*$, where c^* is the complex conjugate of the constant c. In general, however, the ket vector is a complex quantity from which one may not be able to separate the real from the imaginary parts. Thus we call the bra $\langle A|$ the complex imaginary of $|A\rangle$ or $|\overline{A}\rangle$.

We shall define the scalar product between two N dimensional vectors in the same space as

$$\begin{aligned} |A\rangle &= \sum_{i=1}^{N} a_i\,|A_i\rangle \\ |B\rangle &= \sum_{j=1}^{N} b_j|A_j\rangle \end{aligned} \tag{1.1.2}$$

where a_i and b_j are constants and

$$\langle A|B\rangle = \sum_{k=1}^{N} a_k^* b_k \tag{1.1.3}$$

Thus defined, the *scalar product* between two ket vectors generates a number. Of course, the scalar product of the real velocity vector $|V_{(t)}\rangle$ with any of the basic ket vectors $|\hat{V}_{(x)}\rangle$, $|\hat{V}_{(y)}\rangle$ or $|\hat{V}_{(z)}\rangle$ yields the component of $|V_{(t)}\rangle$ in the direction of the basic ket (see Figure 1.1), e.g.

$$\begin{aligned} \langle \hat{V}_{(x)}|V_{(t)}\rangle &= a_{(t)} \\ \langle \hat{V}_{(y)}|V_{(t)}\rangle &= b_{(t)} \\ \langle \hat{V}_{(z)}|V_{(t)}\rangle &= c_{(t)} \end{aligned} \tag{1.1.4}$$

In particular we shall make use of a dual space made up of basic vectors which are defined only by their scalar products with the basic ket vectors of the original space.

For example, choose a set of numbers, the i^{th} one of which we designate by ϕ_i, and each of which is a linear function of a single ket vector $|A_i\rangle$.

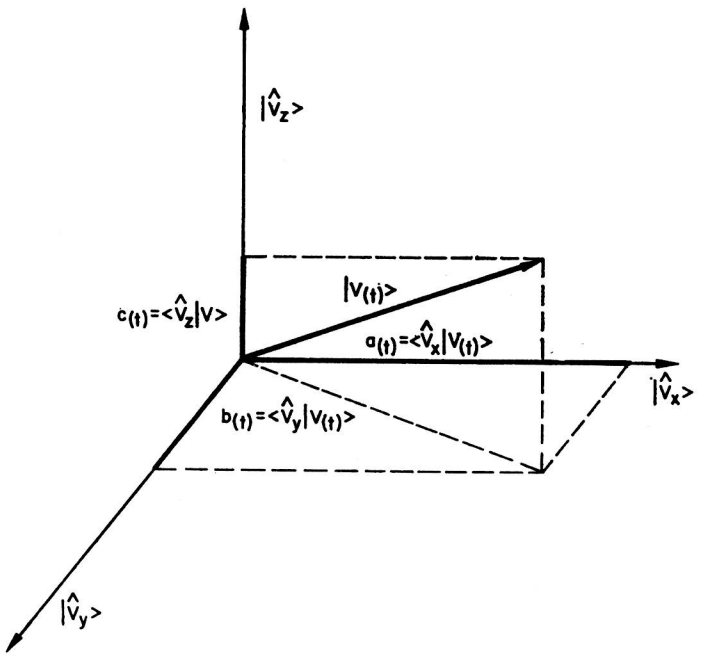

Figure 1.1 The velocity of a system represented as a vector in velocity space.

Each ϕ_i may be looked on as the result of the scalar product of the i^{th} basic ket vector with some bra vector $\langle B_i|$, i.e.,

$$\phi_i = \langle B_i|A_i\rangle \tag{1.5}$$

The set of bra vectors thus generated is the dual space. Our dual space is a linear function of the original ket vectors. As an example, Figure 1.2 shows the relation between a real two dimensional space defined by the basic kets $|\hat{x}\rangle$ and $|\hat{y}\rangle$ and its dual space defined by the basic bras $\langle \hat{B}_1|$ and $\langle \hat{B}_2|$.

The length of a ket vector is as usual defined as the square root of its scalar product with its conjugate bra

$$\langle A|A\rangle^{\frac{1}{2}} = \text{length } |A\rangle \tag{1.1.6}$$

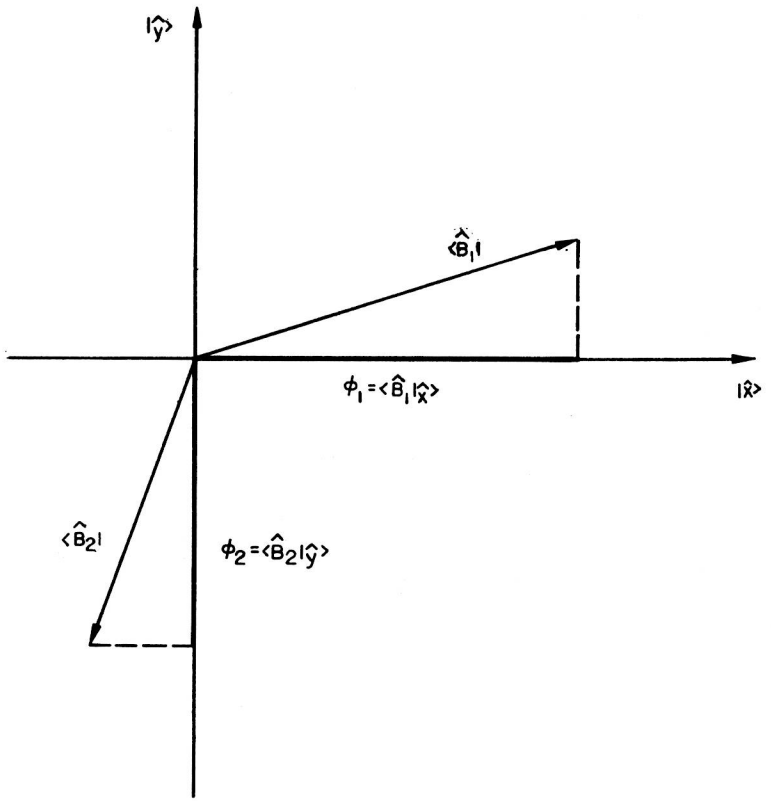

Figure 1.2 Relation between the basic kets $|\hat{x}\rangle$ any $|\hat{y}\rangle$ and the dual space basic vectors $\langle \hat{B}_1|$ and $|\hat{B}_2\rangle$.

In most application, it is convenient to normalize the length of our ket vectors such that

$$\langle A|A\rangle = 1 \tag{1.1.7}$$

1.2 LINEAR OPERATORS

An operator is a quantity that denotes an operation to be performed on a function. An operator α, acting on a ket vector from the left yields a ket that may differ both in magnitude and direction from the original

$$\alpha\,|A_0\rangle = |A\rangle \tag{1.2.1}$$

The operator is always written to the left of the ket.

We will concern ourselves mainly with linear operators. The conditions for linearity may be written

$$\alpha[|A\rangle + |B\rangle] = \alpha\,|A\rangle + \alpha\,|B\rangle \tag{1.2.2}$$

$$\alpha[c\,|A\rangle] = c\alpha\,|A\rangle \tag{1.2.3}$$

where c is a number.

Linear operators may be added

$$[\alpha + \beta]\,|A\rangle = \alpha\,|A\rangle + \beta\,|A\rangle \tag{1.2.4}$$

Multiplication of linear operators e.g. $\alpha\beta$ is carried out by performing first the operation β and then operating on the result with α. The resultant operator $\alpha\beta$ need not be linear.

$$\alpha\beta\,|A\rangle = \alpha[\beta\,|A\rangle] \tag{1.2.5}$$

Let us investigate, for example, the result of the successive operation of the two displacement operators Γ_x and Γ_θ which are defined to produce unit displacement of a vector in the x and θ directions, respectively. As can be seen from Figure 1.3, the order in which the displacements of the vector $\mathbf{R}$ are produced is immaterial, i.e.,

$$\Gamma_x\Gamma_\theta\mathbf{R} = \Gamma_\theta\Gamma_x\mathbf{R} \tag{1.2.6}$$

for the result $\mathbf{R}'$ of the multiplicative operation has the same orientation no matter which order of operation is chosen. However, note that linear operators do not necessarily commute thus their order must be preserved. For example, consider the two independent operations 1. taking a breath and 2. putting your head in a bucket of water. Clearly, performing 2. first

and then 1. yields a quite different result then performing the operations in the opposite order.

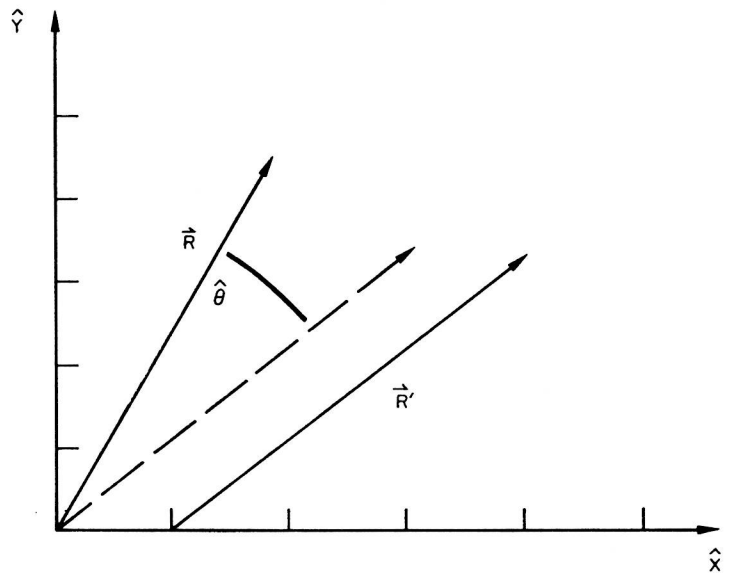

Figure 1.3 The successive operation on **R** with the unit translation operators Γ_x and Γ_θ showing their commutative property.

PROBLEM

(A) Show that the operators

$$\alpha = \frac{\partial}{\partial x} \quad \text{and} \quad \beta = \frac{\partial}{\partial y}$$

commute by operating on the vector

$$\mathbf{A} = \hat{\imath} y^2 z^2 + \hat{\jmath} x^2 z^2 + \hat{k} x^2 y^2$$

(B) Similarly show that

$$\alpha' = x \quad \text{and} \quad \beta' = \partial/\partial x$$

do not commute.

Linear operators may also act on bra vectors and are defined to do so only from the right

$$\overline{[\beta\,|B\rangle]} = \langle B|\,\bar{\beta} \tag{1.2.7}$$

where $\bar{\beta}$ is the adjoint of β.

A linear operator may act on a ket or bra vector in such a way as to produce a vector unchanged in direction but changed only in magnitude

$$\alpha\,|A\rangle = a\,|A\rangle \tag{1.2.8}$$

where a is a constant called the *eigenvalue* of the linear operator α, and the ket $|A\rangle$ is an *eigenket* of α. A similar situation exists for bra vectors.

PROBLEM

Determine if the vector **R**, where

$$\mathbf{R} = \hat{\imath}\,\frac{e^{atx}}{x} + \hat{\jmath}\,\frac{e^{bty}}{y} + \hat{k}\,\frac{e^{ctz}}{z}$$

is an eigenvector of the operator $\partial/\partial t$.

A *real linear operator* is a real operator whose eigenvalues are real numbers. Therefore, as in equation (1.2.8), if α is a real linear operator, a is a real number.

It is easily shown that the eigenvalue a, associated with the eigenket of a real linear operator α is the same as the eigenvalue associated with the eigenbra of the real linear operator $\bar{\alpha}$ by forming the complex imaginary of the eigenvalue equation (1.2.8) which yields

$$\langle A|\,\bar{\alpha} = \langle A|\,a^* \tag{1.2.9}$$

The Orthogonality Theorem

The orthogonality theorem states that two eigenvectors of a real linear operator belonging to different eigenvalues are orthogonal. To prove this we let ξ be a real linear operator, $|A\rangle$ be an eigenket belonging to the eigenvalue a and $|B\rangle$ be an eigenket belonging to the eigenvalue b. Thus we may write the eigenvalue equations

$$\begin{aligned} \xi\,|A\rangle &= a\,|A\rangle \\ \xi\,|B\rangle &= b\,|B\rangle \end{aligned} \tag{1.2.10}$$

Taking the complex imaginary of 1.2.10

$$\langle A|\,\xi = \langle A|\,a \tag{1.2.11}$$

and multiplying by $|B\rangle$ from the right, we find

$$\langle A|\,\xi\,|\beta\rangle = \langle A|\,a\,|B\rangle$$

and

$$\langle A|\,\xi\,|B\rangle = \langle A|\,b\,|B\rangle \tag{1.2.12}$$

Subtracting the equations in (1.2.12) we find

$$\langle A|B\rangle\,(a - b) = 0 \tag{1.2.13}$$

Thus, if $a \neq b$, the scalar product $\langle A|B\rangle$ is equal to zero and the eigenkets

$|A\rangle$ and $|B\rangle$ are orthogonal. When $|A\rangle$ and $|B\rangle$ are orthonormal we can generalize equation (1.2.13) for the case of discrete eigenvalues a and b

$$\langle A|B\rangle = \delta_{a,b} \tag{1.2.14}$$

where $\delta_{a,b}$ is the *Kronecker delta* which has the value 0 for $a \neq b$, and 1 for $a = b$. When $a = b$, $|A\rangle$ and $|B\rangle$ are called *degenerate*.

For the case where we have a continuous range of eigenvalues we may write

$$\langle A'|A''\rangle = \delta(a' - a'') \tag{1.2.15}$$

where $\delta(a' - a'')$ is the *Dirac delta* for continuous eigenvalues and is equal to zero except when $a' = a''$, in which case it has the value 1 and $|A'\rangle$ and $|A''\rangle$ are again degenerate. Note that

$$\int_{-\infty}^{+\infty} \delta_{(a'-a'')} da' = 1 \tag{1.2.16a}$$

and

$$\int_{-\infty}^{+\infty} f_{(x)} \delta_{(x-a)} dx = f_{(a)} \tag{1.2.16b}$$

Observables

Two important assumptions made by Dirac in order to connect his abstract mathematics with experience are that (1) measurable quantities correspond to the eigenvalues of real linear operators. These types of operators are called *observables*. (2) If the eigenvalue of a real linear operator ξ is measurable with the system in a particular state, the act of making a measurement will cause the system to jump into one of a number of allowed states. These states into which the system may jump are assumed to be such that the original state is dependent upon them and thus each must be also an eigenstate of ξ. Thus the original state is dependent on eigenstates of ξ. Since the original state may be any state, we conclude that any state must be dependent on the eigenstates of an observable, and thus an observable must have a complete set of eigenstates, i.e. that any other state be constructable from them. For example, the unit vectors $\hat{\imath}$, $\hat{\jmath}$ and $\hat{k}$ form a complete set in cartesian space since any other cartesian vector may be constructed from a linear combination of these vectors.

Where the eigenvalues of the observable ξ consist of a discrete set of numbers in a certain range such as the energy levels of a harmonic oscillator, the condition that any state $|P\rangle$ is dependent on the complete set of kets $|A_1\rangle$, $|A_2\rangle \ldots |A_i\rangle \ldots |A_n\rangle$ is written

$$|P\rangle = \sum_{i=1}^{n} c_i |A_i\rangle \tag{1.2.17}$$

where c_i is a number.

If the eigenvalues b' of an observable ξ consist of all of the numbers in a certain range, for example the spatial coordinates of an electron, the condition that any ket $|P\rangle$ is dependent on the complete set of kets $|B_1'\rangle, |B_2'\rangle \ldots |B_i'\rangle \cdots |B_n'\rangle$ is expressed

$$|P\rangle = \int |B'\rangle \, \mathrm{d}b' \tag{1.2.18}$$

where we integrate over the range of eigenvalues b' necessary to construct $|P\rangle$.

There may exist a state $|P\rangle$ such that it is dependent upon sets of both discrete and continuous states, in which case we write

$$|P\rangle = \sum_{i=1}^{N} c_i |A_i\rangle + \int |B'\rangle \, \mathrm{d}b' \tag{1.2.19}$$

We shall postulate that if a quantum mechanical system is in an eigenstate $|A\rangle$ of a real linear operator *which* belongs to the eigenvalue a, a measurement of the real linear operator will always give the number a. A real linear operator "which may be measured" is called an *observable* and thus any measurement of an observable must yield one of its eigenvalues.

Therefore the eigenstates of an observable form a complete set since any state is dependent on them. Conversely, any real linear operator whose eigenstates form a complete set is an observable.

We can generate an extremely useful linear operator from a complete set of n discrete or n continuous states. Let us form the sum

$$\sum_{i=1}^{n} |A_i\rangle \langle A_i| \tag{1.2.20}$$

and multiply from the right by the ket $|A_J\rangle$

$$\sum_{i=1}^{n} |A_i\rangle \langle A_i|A_J\rangle = \sum_{i=1}^{n} |A_i\rangle \, \delta_{i,J} = |A_J\rangle \tag{1.2.21}$$