Appendix B

OPERATORS

In this appendix we discuss some topics related to linear operators. The set of admissible wave functions are square integrable functions. Since

$$\psi(x) = \alpha\psi_1(x) + \beta\psi_2(x) \tag{B-1}$$

is square integrable, if $\psi_1(x)$ and $\psi_2(x)$ are square integrable and α, β are arbitrary complex numbers, we say that the ψ's form a *linear space*. An operator A on this space is a mapping:

$$A\psi(x) = \phi(x) \tag{B-2}$$

where $\phi(x)$ is also square integrable. Among all the operators there is a subset called *linear operators*, which have the property that

$$A\alpha\psi(x) = \alpha A\psi(x) \tag{B-3}$$

where α is an arbitrary complex constant, and

$$A[\alpha\psi_1(x) + \beta\psi_2(x)] = \alpha A\psi_1(x) + \beta A\psi_2(x) \tag{B-4}$$

with α, β being complex numbers. A further subset is the *hermitian operators* for which the expectation value for all admissible $\psi(x)$,

$$\langle A\rangle_\psi = \int dx\psi^*(x)\, A\psi(x) \tag{B-5}$$

is real. First we prove that for all admissible ψ_1 and ψ_2

$$\int \psi_2^*(x)\ A\psi_1(x)\ dx = \int [A\psi_2(x)]^*\ \psi_1(x)\ dx \tag{B-6}$$

holds.

The reality of $\langle A \rangle$ implies that

$$\int dx \psi^*(x)\ A\psi(x) = \int dx\ [A\psi(x)]^*\ \psi(x) \tag{B-7}$$

Now substitute for $\psi(x)$

$$\psi(x) = \psi_1(x) + \lambda\psi_2(x) \tag{B-8}$$

This implies that

$$\int dx(\psi_1^* + \lambda^*\psi_2)\ A(\psi_1 + \lambda\psi_2) = \int dx(\psi_1 + \lambda\psi_2)(A\psi_1 + \lambda A\psi_2)^* \tag{B-9}$$

Using hermiticity, that is,

$$\int dx \psi_i^* A\psi_i = \int dx \psi_i (A\psi_i)^* \qquad i = 1.2 \tag{B-10}$$

we obtain

$$\lambda^* \int \psi_2^* A\psi_1 + \lambda \int \psi_1^* A\psi_2 = \lambda \int \psi_2 (A\psi_1)^* + \lambda^* \int \psi_1 (A\psi_2)^* \tag{B-11}$$

Since λ is an arbitrary complex number, the relations for the coefficient of λ and for the coefficient of λ^* must separately hold. Thus

$$\int dx \psi_2^* A\psi_1 = \int dx(A\psi_2)^*\ \psi_1 \tag{B-12}$$

The next result that we wish to prove is that *eigenfunctions of a hermitian operator corresponding to different eigenvalues are orthogonal.* Consider the two equations

$$A\psi_1(x) = a_1\psi_1(x)$$

and

$$[A\psi_2(x)]^* = a_2\psi_2^*(x) \tag{B-13}$$

Note that a_2 is real since the eigenvalues of a hermitian operator are real. Take the scalar product of the first equation with ψ_2^* and the second equation with ψ_1. Thus

$$\begin{aligned} \int dx \psi_2^* A\psi_1(x) &= a_1 \int \psi_2^*(x)\ \psi_1(x)\ dx \\ \int dx(A\psi_2)^*\ \psi_1(x) &= a_2 \int \psi_2^*(x)\ \psi_1(x)\ dx \end{aligned} \tag{B-14}$$

Subtracting, we get

$$(a_1 - a_2) \int \psi_2^*(x)\ \psi_1(x)\ dx = \int dx \psi_2^* A \psi_1 - \int dx (A\psi_2)^*\ \psi_1 \\ = 0 \tag{B-15}$$

Thus, if $a_1 \neq a_2$, we have

$$\int \psi_2^*(x)\ \psi_1(x)\ dx = 0 \tag{B-16}$$

If we define the hermitian conjugate of the operator A by $A^\dagger$, so that

$$\int dx (A\psi_2)^*\ \psi_1 \equiv \int dx \psi_2^* A^\dagger \psi_1 \tag{B-17}$$

then for a hermitian operator

$$A = A^\dagger \tag{B-18}$$

We can prove that

$$(AB)^\dagger = B^\dagger A^\dagger \tag{B-19}$$

To do so, we note that

$$\begin{aligned} \int \psi_2^* (AB)^\dagger\ \psi_1 &= \int (AB\psi_2)^* \psi_1 \\ &= \int (B\psi_2)^*\ (A^\dagger \psi_1) \\ &= \int \psi_2^* B^\dagger (A^\dagger \psi_1) \\ &= \int \psi_2^* B^\dagger A^\dagger \psi_1 \end{aligned} \tag{B-20}$$

A generalization of this is

$$(ABC \cdots Z)^\dagger = Z^\dagger \cdots C^\dagger B^\dagger A^\dagger \tag{B-21}$$

Thus, a product of two hermitian operators is only hermitian if the two operators commute:

$$(AB)^\dagger = B^\dagger A^\dagger = BA = AB + [B, A] \tag{B-22}$$

Another result is that for any operator A, the following

$$\begin{gathered} A + A^\dagger \\ i(A - A^\dagger) \\ AA^\dagger \end{gathered} \tag{B-23}$$

will be hermitian.

Next we prove the "uncertainty relations." We define

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 = \langle (A - \langle A \rangle)^2 \rangle \tag{B-24}$$

Let

$$\begin{aligned} U &= A - \langle A \rangle \\ V &= B - \langle B \rangle \end{aligned} \tag{B-25}$$

and consider

$$\phi = U\psi + i\lambda V\psi \tag{B-26}$$

Then

$$I(\lambda) = \int dx \phi^* \phi \geq 0 \tag{B-27}$$

With A and B hermitian, so are U and V. We may thus rewrite:

$$\begin{aligned} I(\lambda) &= \int dx (U\psi + i\lambda V\psi)^* \, (U\psi + i\lambda V\psi) \\ &= \int dx (U\psi)^* \, (U\psi) + \lambda^2 \int dx (V\psi)^* \, (V\psi) \\ &\quad + i\lambda \int dx [(U\psi)^* \, (V\psi) - (V\psi)^* \, (U\psi)] \\ &= \int dx \psi^* (U^2 + \lambda^2 V^2 + i\lambda [U, V]) \psi \\ &= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \int dx \psi^* \, [U, V] \, \psi \geq 0 \\ &= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \, \langle [A, B] \rangle \end{aligned} \tag{B-28}$$

The minimum will occur when

$$2\lambda (\Delta B)^2 + i \langle [A, B] \rangle = 0 \tag{B-29}$$

Substituting the solution

$$\lambda = -i \frac{\langle [A, B] \rangle}{2 \, (\Delta B)^2} \tag{B-30}$$

into $I(\lambda)$, we get

$$(\Delta A)^2 - \frac{\langle [A, B] \rangle^2}{4 (\Delta B)^2} + \frac{\langle [A, B] \rangle^2}{2 (\Delta B)^2} \geq 0$$

that is,

$$(\Delta A^2) \, (\Delta B)^2 \geq \tfrac{1}{4} \, \langle i [A, B] \rangle^2 \tag{B-31}$$

lly, the minimum value occurs when ψ is such that $U\psi$ and $V\psi$ are pro- to each other. For the case of the operators x and p, this means that

$$\frac{\hbar}{i}\frac{d\psi(x)}{dx} + i\beta x\psi(x) = 0 \tag{B-32}$$

whose solution is

$$\psi(x) = C\, e^{-\beta(x^2/2\hbar)} \tag{B-33}$$

a ground-state eigenfunction of the harmonic oscillator. It is important to note that the uncertainty relation

$$(\Delta A)^2\, (\Delta B)^2 \geq \tfrac{1}{4}\, (\langle i[A,\, B]\rangle)^2 \tag{B-34}$$

was derived without any use of wave concepts or the reciprocity between a wave form and its Fourier transform. The results depends entirely on the operator properties of the observables A and B.

We conclude the appendix by listing some properties of commutators.

(i)

$$[A,\, B] = -\,[B,\, A] \tag{B-35}$$

(ii)

$$\begin{aligned}[A,\, B]^\dagger &= (AB)^\dagger - (BA)^\dagger \\ &= B^\dagger A^\dagger - A^\dagger B^\dagger \\ &= [B^\dagger,\, A^\dagger]\end{aligned} \tag{B-36}$$

(iii) If A and B are hermitian, so is $i[A, B]$. This follows directly from the preceding properties.

(iv)

$$\begin{aligned}[AB,\, C] &= ABC - CAB \\ &= ABC - ACB + ACB - CAB \\ &= A[B,\, C] + [A,\, C]\, B\end{aligned} \tag{B-37}$$

(v) It may be shown term by term that

$$e^A B e^{-A} = B + [A,\, B] + \frac{1}{2!}\,[A,[A,\, B]] + \frac{1}{3!}\,\big[A,[A,[A,\, B]]\big] + \cdots \tag{B-38}$$

This is known as the Baker-Hausdorff lemma and is of some utility in manipulations of operators.

(vi) It is easily established that

$$[A,[B, C]] + [B,[C, A]] + [C,[A, B]] = 0 \tag{B-39}$$

This is called the Jacobi identity.

A more extensive discussion of operators and the linear spaces that they are defined on may be found in J. D. Jackson, *Mathematics for Quantum Mechanics*, W. A. Benjamin, New York, 1962.