**Hermitian Operators**

As mentioned previously, the expectation value of an operator $\hat{A}$ is given by

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| \begin{displaymath} <A> = \int \psi^{*}({\bf r}) \hat{A} \psi({\bf r}) d{\bf r} \end{displaymath} | (55) |

and all physical observables are represented by such expectation values. Obviously, the value of a physical observable such as energy or density must be real, so we require $<A>$ to be real. This means that we must have $<A> = <A>^{*}$, or

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| \begin{displaymath} \int \psi^{*}({\bf r}) \hat{A} \psi({\bf r}) d{\bf r} = \int (\hat{A} \psi({\bf r}))^{*} \psi({\bf r}) d{\bf r} \end{displaymath} | (56) |

Operators $\hat{A}$ which satisfy this condition are called *Hermitian*. One can also show that for a Hermitian operator,

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| \begin{displaymath} \int \psi_1^{*}({\bf r}) \hat{A} \psi_2({\bf r}) d{\bf r} = \int (\hat{A} \psi_1({\bf r}))^{*} \psi_2({\bf r}) d{\bf r} \end{displaymath} | (57) |

for any two states $\psi_1$ and $\psi_2$.

An important property of Hermitian operators is that their eigenvalues are real. We can see this as follows: if we have an eigenfunction of $\hat{A}$ with eigenvalue $a$, i.e. $\hat{A} \psi_a = a \psi_a$, then for a Hermitian operator $\hat{A}$

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| $\displaystyle \int \psi_a^{*} \hat{A} \psi_a$ | $\textstyle =$ | $\displaystyle \int \psi_a (\hat{A} \psi_a)^{*}$ | (58) |
| $\displaystyle a \int \psi_a^{*} \psi_a$ | $\textstyle =$ | $\displaystyle a^{*} \int \psi_a \psi_a^{*}$ |  |
| $\displaystyle (a - a^{*}) \int \vert\psi_a\vert^2$ | $\textstyle =$ | $\displaystyle 0$ |  |

Since $\vert\psi_a\vert^2$ is never negative, we must have either $a = a^{*}$ or $\psi_a = 0$. Since $\psi_a = 0$ is not an acceptable wavefunction, $a = a^{*}$, so $a$ is real.

Another important property of Hermitian operators is that their eigenvectors are orthogonal (or can be chosen to be so). Suppose that $\psi_a$ and $\psi_b$ are eigenfunctions of $\hat{A}$ with eigenvalues $a$ and $b$, with $a \neq b$. If $\hat{A}$ is Hermitian then

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| $\displaystyle \int \psi_a^{*} \hat{A} \psi_b$ | $\textstyle =$ | $\displaystyle \int \psi_b (\hat{A} \psi_a)^{*}$ | (59) |
| $\displaystyle b \int \psi_a^{*} \psi_b$ | $\textstyle =$ | $\displaystyle a^{*} \int \psi_b \psi_a^{*}$ |  |
| $\displaystyle (b - a) \int \psi_a^{*} \psi_b$ | $\textstyle =$ | $\displaystyle 0$ |  |

since $a = a^{*}$ as shown above. Because we assumed $b \neq a$, we must have $\int \psi_a^{*} \psi_b = 0$, i.e. $\psi_a$ and $\psi_b$ are orthogonal. Thus we have shown that eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal. In the case of degeneracy (more than one eigenfunction with the same eigenvalue), we can *choose* the eigenfunctions to be orthogonal. We can easily show this for the case of two eigenfunctions of $\hat{A}$ with the same eigenvalue. Suppose we have

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| $\displaystyle \hat{A} \psi_j$ | $\textstyle =$ | $\displaystyle j \psi_j$ | (60) |
| $\displaystyle \hat{A} \psi_k$ | $\textstyle =$ | $\displaystyle j \psi_k$ |  |

We now want to take linear combinations of $\psi_j$ and $\psi_k$ to form two new eigenfunctions $\psi_{j'}$ and $\psi_{k'}$, where $\psi_{j'} = \psi_j$ and $\psi_{k'} = \psi_k + c \psi_j$. Now we want $\psi_{j'}$ and $\psi_{k'}$ to be orthogonal, so

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| $\displaystyle \int \psi_{j'}^{*} \psi_{k'}$ | $\textstyle =$ | $\displaystyle 0$ | (61) |
| $\displaystyle \int \psi_j^{*} (\psi_k + c \psi_j)$ | $\textstyle =$ | $\displaystyle 0$ |  |
| $\displaystyle \int \psi_j^{*} \psi_k + c \int \psi_j^{*} \psi_j$ | $\textstyle =$ | $\displaystyle 0$ |  |

Thus we merely need to choose

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| \begin{displaymath} c = -\frac{\int \psi_j^{*} \psi_k}{\int \psi_j^{*} \psi_j} \end{displaymath} | (62) |

and we obtain orthogonal eigenfunctions. This Schmidt-orthogonalization procedure can be extended to the case of n-fold degeneracy, so we have shown that for a Hermitian operator, the eigenvectors can be made orthogonal.