Appendix 5: Unitary Operators, the Evolution Operator, the Schrödinger and the Heisenberg Pictures, and Wigner's Formula

A5.1 Unitary Operators, the Evolution Operator

In ordinary 3-dimensional space, there are operators, such as an operator that simply rotates vectors, which alter ordinary vectors while preserving their lengths. Unitary operators do much the same thing in *n*-dimensional complex spaces.[1] Let us start with some definitions. Given an operator (matrix) *A*, its inverse A^{-1} is such that

$$AA^{-1} = A^{-1}A = I.^{2} \qquad \text{(A5.1.1)}$$

An operator (matrix) *U* is *unitary* if its inverse is equal to its Hermitian conjugate (its adjoint), so that

$$U^{-1} = U^{+}, \qquad \text{(A5.1.2)}$$

and therefore

$$UU^{+} = U^{+}U = I. \qquad \text{(A5.1.3)}$$

Since the evolution operator $U(t,t_0)$ and TDSE do the same thing, $U(t,t_0)$ must preserve normalization and therefore unsurprisingly it can be shown that the evolution operator is unitary. Moreover,

$$U(t_n,t_i) = U^{+}(t_i,t_n) = U^{-1}(t_i,t_n). \qquad \text{(A5.1.4)}$$

In addition,

$$U(t_n,t_1) = U(t_n,t_{n-1})U(t_{n-1},t_{n-2})\cdots U(t_2,t_1), \qquad \text{(A5.1.5)}$$

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[1] As we know, the state vector is normalized (has length one), and stays normalized. Hence, the only way for it to undergo linear change is to rotate in *n*-dimensional space.

[2] It is worth noticing that a matrix has an inverse if and only if its determinant is different from zero.

that is, the evolution operator for the system's transition in the interval $t_n - t_1$ is equal to the product of the evolution operators in the intermediate intervals.

A5.2 The Schrödinger and the Heisenberg Pictures, and Wigner's Formula

There are several physically equivalent versions of quantum theory. In the Schrödinger version, systems are described by state vectors whose temporal development is governed by the evolution operator $U(t, t_0)$. While state vectors undergo temporal change, the operators representing observables do not. In the Heisenberg version, the roles are reversed: while the state vectors remains constant in time, the operators undergo temporal change according to the Heisenberg Equation, of which more later. To see how this can be achieved, we need to look a bit more closely at unitary operators.

Unitary operators preserve some interesting properties of the vectors and operators they are applied to. Given a vector $|\psi\rangle$ and a unitary operator *U*,

$$|\widehat{\psi}\rangle = U|\psi\rangle \qquad \text{(A5.2.1)}$$

is the *transform* of $|\psi\rangle$. It turns out that given any two vectors,

$$\langle\psi|\phi\rangle = \langle\widehat{\psi}|\widehat{\phi}\rangle, \qquad \text{(A5.2.2)}$$

which entails that *U* preserves both the norm and the orthogonality of vectors. Moreover, if $\{e_1, ..., e_n\}$ is a basis for space *H*, then $\{\widehat{e}_1, ..., \widehat{e}_n\}$ is a basis for *H* as well. In sum, the transforms of an orthonormal basis constitute another orthonormal basis in the same space.

Having considered some of the properties of the transforms of vectors, we now turn to those of the transforms of operators. By definition, the transform of an operator *O* is the operator $\widehat{O}$ that in the transform basis $\{\widehat{e}_1,...,\widehat{e}_n\}$ has the very same elements O has in the original basis $\{e_1,...,e_n\}$. In other words,

$$\langle \widehat{e}_i|\widehat{O}|\widehat{e}_j\rangle = \langle e_i|O|e_j\rangle. \qquad \text{(A5.2.3)}$$

By working on the left side of (A5.2.3), keeping in mind the relations between bras and kets, and using (A5.2.1), we obtain

$$\langle \widehat{e}_i|\widehat{O}|\widehat{e}_j\rangle = \langle e_i|U^+\widehat{O}U|e_j\rangle = \langle e_i|O|e_j\rangle, \qquad \text{(A5.2.4)}$$

so that

$$U^+\widehat{O}U = O. \qquad \text{(A5.2.5)}$$

By multiplying both sides first on the left by U, and then on the right by $\tilde{U}^*$, we obtain

$$UU^+\widehat{O}UU^+ = UOU^+. \qquad \text{(A5.2.6)}$$

Since U is unitary, we have

$$UU^{-1}\widehat{O}UU^{-1} = \widehat{O} = UOU^+ = UOU^{-1}. \qquad \text{(A5.2.7)}$$

In other words, the transform of an operator is obtained by sandwiching it between U and U^+ or, which is the same, between U and U^{-1}. It turns out that the eigenvectors of $\widehat{O}$ are the transforms of the eigenvectors of O and that the eigenvalues of $\widehat{O}$ and O are the same.

As we know, quantum mechanical predictions are couched in terms of scalar products or matrix elements of density operators. However, as we just saw, these quantities are invariant as long as the same unitary transformation is performed on both kets and operators. Furthermore, we know that the evolution operator is unitary. We have now the ingredients for going from the Schrödinger to the Heisenberg picture. We need to choose a unitary transformation that makes the transform of the time dependent

Schrödinger ket $|\Psi_S(t)\rangle$ the Heisenberg time independent ket $|\Psi_H\rangle$. Let us choose $U^+(t,t_0)=U^{-1}(t,t_0)$ as our unitary operator. Then,

$$|\Psi_H\rangle = U^+(t,t_0)|\Psi_S(t)\rangle = U^+(t,t_0)U(t,t_0)|\Psi_S(t_0)\rangle = |\Psi_S(t_0)\rangle. \qquad \text{(A5.2.8)}$$

In other words, the Heisenberg state vector does not change with time and is equal to the Schrödinger state vector at time zero. The Heisenberg transform of the time independent Schrödinger operator O_S becomes

$$O_H(t) = U^+(t,t_0)O_S U(t,t_0), \qquad \text{(A5.2.9)}$$

which is usually time dependent.

It can be shown that the temporal evolution of a Heisenberg operator $O_H(t)$ is given by the Heisenberg equation

$$i\hbar\frac{d}{dt}O_H(t) = [O_H(t), H_H(t)] + i\hbar\frac{\partial}{\partial t}O_H(t). \qquad \text{(A5.2.10)}$$

So, when the system is conservative (the Hamiltonian H_H is time independent) and the operator commutes with the Hamiltonian (that is, it is a constant of the motion), then (A5.2.10) becomes

$$i\hbar\frac{d}{dt}O_H(t) = 0, \qquad \text{(A5.2.11)}$$

that is, $O_H(t)$ is (not surprisingly) time invariant. Moreover, in this case $O_S = O_H(t)$, that is, the Schrödinger and the Heisenberg operators are identical.

Wigner's formula is usually couched in terms of Heisenberg projectors, the transforms of the corresponding Schrödinger projectors according to the formula

$$W = \hat{P} = U^{-1}(t'',t')PU(t'',t') = U(t',t'')PU(t'',t'), \qquad \text{(A5.2.12)}$$

where t'' is the time of the measurement being considered and t' that of the previous one. Wigner's formula is then given by

$$\Pr\left(a_i, b_j, \ldots, f_p, g_q\right) = Tr\left(W_q^G W_p^F \cdots W_j^B W_i^A \rho W_i^A W_j^B \cdots W_p^F W_q^G\right), \qquad \text{(A5.2.13)}$$

where ρ is the density operator at time zero, that is when a_i is obtained.[3]

[3] Note that the projectors corresponding to the earlier measurements are inside.

Exercises

Exercise A5.1

Show that $UU^{+} = U^{+}U = I$.

Exercise A5.2

Show that $\langle \psi_1 | \psi_2 \rangle = \langle \widehat{\psi}_1 | \widehat{\psi}_2 \rangle$.

Answers to the Exercises

Exercise A5.1

Since $U^{-1} = U^{+}, UU^{+} = U^{+}U = I$.

Exercise A5.2

$\left\langle \widehat{\psi}_1 \middle| \widehat{\psi}_2 \right\rangle = \left\langle \psi_1 U^{+} \middle| U\psi_2 \right\rangle = \left\langle \psi_1 \middle| I\psi_2 \right\rangle = \left\langle \psi_1 \middle| \psi_2 \right\rangle$.