The Unitarity of the U Operator

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The U operator, which connects state vectors in interaction representation for different times, can be applied meaningfully to asymptotic values of state vectors $\Phi(\pm\infty)$ if these limits exist. The conditions for this occurrence are stated for the simplest case. If the restriction resulting from the definition of the asymptotic values is respected, all U operators are unambiguously unitary. A more general operator W which can act on all state vectors, can be defined, but it is not unitary.

THE operator $U(t,\tau)$, defined in interaction representation by

$$\Phi(t)=U(t,\tau)\Phi(\tau), \tag{1}$$

is known to be unitary for finite times t, τ, but some doubt and disagreement exists concerning the limits $U(t,-\infty)$ and $U(\infty,\tau)$.[1,2] It will be shown that these operators have, by their definition, a severely restricted domain, but that they are unambiguously unitary if this restriction is respected.

$U(t,-\infty)$ is defined by

$$\Phi(t)=U(t,-\infty)\lim_{\tau\to-\infty}\Phi(\tau) \tag{2}$$

and $U(\infty,t)$ by

$$\lim_{\tau\to\infty}\Phi(\tau)=U(\infty,t)\Phi(t). \tag{3}$$

$U(t,-\infty)$ has meaning only if its domain is restricted to those state vectors which tend to a limit at $-\infty$, and $U(\infty,t)$ only if its range is restricted to such Φ's which tend to a limit for $+\infty$.

Let the Hamiltonian be $H=K+V$, where V is the interaction term. If $\Phi(\pm\infty)$ are to have limits, the corresponding Schrödinger wave functions must behave asymptotically like

$$\Psi\xrightarrow[\tau\to\pm\infty]{} e^{-iKt}\psi_\pm(x), \tag{4}$$

where $\psi_\pm(x)$ is time-independent. This will happen only if Ψ is entirely outside the range of interaction for the distant future (past), for then

$$\lim_{t\to\pm\infty} V\Psi(t)=0,$$

and the Schrödinger equation leads to the form (4). The explicit conditions for this behavior will now be indicated.

If Ψ is represented as a wave packet,

$$\Psi(x,t)=\int C(E)\psi_E(x)e^{-iEt}dE, \tag{5}$$

where $\psi_E(x)$ are eigenfunctions of $K+V$, then in virtue of well-known properties of the Fourier integral, $\Psi(x,t)$ tends to zero in any finite region of x as t becomes $\pm\infty$ if $C(E)\Psi_E$ is absolutely integrable, and in particular contains no delta function belonging to bound states. Hence, in the distant past and distant future this wave function will be entirely outside the range of the potential. The essential limitation for the domains and ranges $U(t,-\infty)$ and $U(\infty,t)$ is, therefore, the absence of an admixture of bound states.

Since the ranges and domains of the two operators $U(t,-\infty)$ and $U(\infty,t)$ are identical, it is legitimate to extend the well-known relation

$$U(t,t_0)=U(t,t')U(t',t_0) \tag{6}$$

to

$$S=U(\infty,-\infty)=U(\infty,0)U(0,-\infty). \tag{7}$$

Since the operators for infinite times differ in their action only infinitesimally from operators for large times, the unitarity of the U and S operators can be now inferred from the known property of these operators for finite times, as long as the restriction on domain is respected. To express the U operators in terms of time-independent solutions of the Schrödinger equation, one can follow the same procedure as Ma,[1] keeping in mind that with respect to the domain considered, the positive-energy solutions ψ_λ form a complete system. Hence,

$$\int \psi_\lambda\psi_\lambda{}^*d\lambda=1, \tag{8}$$

and the unitarity of the U operators is thus confirmed. An entirely different operator is defined by

$$\begin{aligned} W(\infty,t)&=\lim_{\tau\to\infty}U(\tau,t),\\ W(t,-\infty)&=\lim_{\tau\to-\infty}U(t,\tau), \end{aligned} \tag{9}$$

with a range (domain) containing all squared-integrable functions. One will require that W should be identical with U within the restricted domain, but otherwise the manner in which limits for indefinitely oscillating matrix elements are defined, is arbitrary. There seems to be no real necessity for defining such an operator, but we can see two motivations for doing so.

[1] S. T. Ma, Phys. Rev. **87**, 652 (1952).
[2] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

(a) The replacement of oscillatory functions by their asymptotic mean value is a procedure often used in physics and very successfully applied by Gell-Mann and Goldberger for explicit evaluations.[2] This can be done in the present case either by formal handling of "conditional equalities"[1] or by an explicit prescription which is equivalent to a "dc filtering" of the asymptotic values.[2]

(b) One can think of situations where the initial state is a linear combination of bound and positive-energy states, i.e., an atom the nucleus of which undergoes instantaneous conversion: immediately afterward, the state of the electrons is a mixture of bound and free states of the Hamiltonian describing the nucleus with altered charge. In this case, one would decompose the Schrödinger wave function $\Psi(0)$ into $\Psi_{\text{bound}}+\Psi_{\text{free}}$ and the asymptotic form is

$$\Psi \underset{t\to\infty}{\longrightarrow} e^{-iKt}U(\infty,0)\Psi_{\text{free}}(0)+e^{-i(K+V)t}\Psi_{\text{bound}}(0). \quad (10)$$

It is advantageous now to define an operator $W(\infty,0)$ so that it annuls the bound state part of $\Psi(0)$, i.e.,

$$W(\infty,0)\Psi_{\text{bound}}=0, \quad (11)$$

because it is then unnecessary to decompose $\Psi(0)$ and one obtains immediately the scattered part of the wave function

$$\Psi_{sc} \underset{t\to\infty}{\longrightarrow} e^{-iKt}W(\infty,0)\Psi(0). \quad (12)$$

It is remarkable that the additional requirement (11) leads precisely to the same operator as the one obtained by the limiting procedures discussed under (a), although the motivation for its introduction is entirely different.

It should be noted that these remarks, as well as most of the previous work on the time-dependent scattering, applies only to the simplest case where the incident system is identical with the scattered one. Different considerations are required for multichannel processes.