Bound States and the Interaction Representation

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The temporal development of the state vectors in the interaction representation is investigated for a quantum-mechanical system that has bound states. It is shown that there is a non-unitary operator which determines the variation of the state vectors of the free states. This operator satisfies the same differential equation and initial condition as the unitary operator which transforms a state vector at the remote past to the state vector at a finite time or in the remote future. The present investigation is relevant to a remark made by H. S. Snyder.

No iteration process is made use of in the general investigation. Born's method of successive approximations is discussed at the end.

I. INTRODUCTION

THE connection between the time-independent (stationary)[1] and the time-dependent (nonstationary)[2] formulations of the theory of scattering has been investigated by several authors.[3,3a] Snyder has pointed out that further clarification is needed for obtaining complete consistency in such theoretical considerations in the case of a quantum-mechanical system that has bound states. It is the purpose of the present note to contribute some discussions relevant to this question.

Our discussions also throw some light on the relativistic two-body problem[4] and the general theory of the bound states.[5]

II. TEMPORAL DEVELOPMENT OF THE STATE VECTORS IN THE INTERACTION REPRESENTATION

The time-dependent theory of scattering is usually developed in the interaction representation with the σ-surfaces taken to be planes. In this section such a time-dependent theory will be extended to include the bound states. We shall take the time-independent formulation of quantum mechanics as our starting point.

We consider a quantum-mechanical system with the following properties. The Hamiltonian of the system is of the form

$$H=H_0+H_1, \tag{1}$$

where H_0 is the Hamiltonian of the free particles and H_1 is the interaction of the particles. There is no time-dependent external force, so that in the Schrödinger picture H_0 and H_1 are time-independent. The free-particle Hamiltonian H_0 has real eigenvalues that form one or several continuous spectra. The total Hamiltonian H has the same continuous spectra of eigenvalues and also discrete eigenvalues which have no one-to-one correspondence to the eigenvalues of H_0. The continuous eigenvalues of H correspond to the energies of the hyperbolic orbits in the classical theory; the discrete eigenvalues correspond to the energies of the elliptic orbits: The eigenstates of H with continuous and discrete eigenvalues will be referred to as the free and bound states, respectively.[5a]

Let us first state the basic features of the time-independent theory of such a quantum-mechanical system. Greek and Latin indices will be used to denote the free and bound states, respectively. Let ψ and ϕ be the eigenvectors of H and H_0, respectively. We have then

$$H\psi_\lambda=E_\lambda\psi_\lambda, \tag{2}$$

$$H_0\phi_\lambda=E_\lambda\phi_\lambda, \tag{3}$$

$$H\psi_s=E_s\psi_s. \tag{4}$$

The ψ's and ϕ's each form a complete orthonormal set of eigenvectors. There is no ϕ corresponding to ψ_s, but there is a one-to-one correspondence between the

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[1] W. Heisenberg, Z. Physik **1**, 608 (1946); C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **23**, No. 1 (1945); **22**, No. 19 (1946); W. Pauli, *Meson Theory of Nuclear Forces* (Interscience Publishers, New York, 1948); G. Wentzel, Revs. Modern Phys. **19**, 1 (1947).

[2] W. Heitler, *Quantum Theory of Radiation* (Oxford University Press, London, 1944); E. C. G. Stueckelberg, Helv. Phys. Acta **18**, 195 (1945); S. Tomonaga, Prog. Theoret. Phys. **1**, 27 (1946); J. Schwinger, Phys. Rev. **74**, 1439 (1948); R. P. Feynman, Phys. Rev. **76**, 749, 769 (1949); F. J. Dyson, Phys. Rev. **75**, 486, 1736 (1949); D. Rivier, Helv. Phys. Acta **22**, 265 (1949); K. O. Friedrichs, Commun. Pure Appl. Math. **5**, 1 (1952).

[3] K. O. Friedrichs, Commun. Pure Appl. Math. **1**, 361 (1948); B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950); H. S. Snyder, Phys. Rev. **83**, 1154 (1951); M. Schoenberg, Nuovo cimento **8**, 403, 651 (1951); E. Arnous and S. Zienau, Helv. Phys. Acta **24**, 279 (1951); J. Pirenne, Phys. Rev. **86**, 395 (1952).

[3a] For those problems in which the initial condition is specified for $t=0$ rather than $t=-\infty$, the connection between the two formulations has been investigated by W. Heitler and S. T. Ma, Proc. Irish Academy **52** A, No. 9, 109 (1949); E. Arnous and S. Zienau (see reference 3); M. Schoenberg, Nuovo cimento **8**, 817 (1951).

[4] Y. Nambu, Prog. Theoret. Phys. **5**, 82 (1950); E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951); J. Schwinger, Proc. Natl. Acad. Sci. **37**, 452, 455 (1951); M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951); M. Jean, Compt. rend. **233**, 602 (1951).

[5] B. Ferretti, Nuovo cimento **8**, 108 (1951); F. J. Dyson, Phys. Rev. **82**, 428 (1951); **83**, 608, 1207 (1951); K. Nishijima, Prog. Theoret. Phys. **6**, 37 (1951).

[5a] For a discussion of the identity of the continuous spectra of H_0 and H_1, see P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, London, 1947). The discrete eigenvalues of H are assumed to be real and outside the range of the continuous spectra. Note the difference between the meanings of the word "free" for "free particles" in connection with H_0 and "free state" in connection with H.

ψ_λ and ϕ_λ. Put

$$\psi_\lambda = W\phi_\lambda. \tag{5}$$

The quantities

$$(\phi_\mu, \psi_\lambda) = (\phi_\mu, W\phi_\lambda) = (\mu|W|\lambda) \tag{6}$$

form a matrix which Møller calls the wave matrix. It satisfies the equation

$$(E_\lambda - E_\mu)(\mu|W|\lambda) = (\mu|H_1 W|\lambda). \tag{7}$$

The radiation conditions for ψ_λ to describe plane incident waves together with spherical outgoing or ingoing waves give the solutions

$$(\mu|W_\pm|\lambda) = \delta(\mu-\lambda) \mp 2\pi i \delta_\pm(E_\lambda - E_\mu)(\mu|H_1 W_\pm|\lambda), \tag{8}$$

where

$$\delta_\pm(\omega) = \tfrac{1}{2}\delta(\omega) \pm (i/2\pi)(P/\omega), \tag{9}$$

with P denoting the principal value. The S-matrix is given by

$$(\mu|S|\lambda) = \delta(\mu-\lambda) - 2\pi i \delta(E_\lambda - E_\mu)(\mu|H_1 W_+|\lambda). \tag{10}$$

For the bound states we have

$$(E_s - E_\mu)(\phi_\mu, \psi_s) = (\phi_\mu, H_1\psi_s), \tag{11}$$

which gives

$$(\phi_\mu, \psi_s) = \frac{1}{E_s - E_\mu}(\phi_\mu, H_1\psi_s). \tag{12}$$

There is no singularity in Eq. (12) as in Eq. (8). The orthogonality conditions for ψ_λ and ψ_s give rise to the conditions

$$(\psi_s, W_\pm\phi_\lambda) = 0 \tag{13}$$

or simply

$$\left.\begin{aligned} \psi_s^\dagger W_\pm &= 0, \\ W_\pm^\dagger \psi_s &= 0, \end{aligned}\right\}, \tag{14}$$

where we use the sign $\dagger$ to denote the Hermitian conjugate of an operator or the conjugate imaginary of an eigenvector.

As Møller has shown, the orthonormal condition for the $\psi_{+\lambda}$ and the completeness relation

$$\int \psi_{+\lambda}\psi_{+\lambda}^\dagger d\lambda + \sum \psi_s \psi_s^\dagger = 1 \tag{15}$$

lead to the following relations for W_+:

$$W_+^\dagger W_+ = 1, \tag{16}$$

$$W_+ W_+^\dagger = 1 - \sum \psi_s \psi_s^\dagger. \tag{17}$$

The basic equations of the time-dependent theory are mathematical consequences of the above equations. Friedrichs has dealt with the temporal development of the wave matrix by means of the theory of spectral representation. It may be of general interest to have a mathematical treatment using a language more familiar to physicists.

In the Schrödinger picture the state vector that is equal to $\psi_{\pm\lambda}$ at $t=0$ is equal to $\psi_{\pm\lambda}\exp(-iE_\lambda t)$ for an arbitrary value of t. It is therefore given by

$$\psi_{\pm\lambda}(t) = \exp[i(H_0 - E_\lambda)t]\psi_{\pm\lambda} \tag{18}$$

in the interaction representation. It follows from Eqs. (5) and (18) that

$$\psi_{\pm\lambda}(t) = W_\pm(t)\phi_\lambda, \tag{19}$$

where

$$W_\pm(t) = \exp(iH_0 t) W_\pm \exp(-iH_0 t) \tag{20}$$

satisfies the equation

$$i(dW_\pm(t)/dt) = H_1(t) W_\pm(t), \tag{21}$$

with

$$H_1(t) = \exp(iH_0 t) H_1 \exp(-iH_0 t). \tag{22}$$

Using the relations[6]

$$\lim_{t\to\pm\infty} \delta_+(\omega)\exp(-i\omega t) = \begin{cases} \delta(\omega) \\ 0 \end{cases}, \tag{23}$$

$$\lim_{t\to\pm\infty} \delta_-(\omega)\exp(-i\omega t) = \begin{cases} 0 \\ \delta(\omega) \end{cases}, \tag{24}$$

we have

$$W_+(-\infty) = 1, \tag{25}$$

$$W_+(\infty) = S, \tag{26}$$

$$W_-(\infty) = 1. \tag{27}$$

Using the relations

$$\int_{-\infty}^{t} \exp(-i\omega t')dt' = 2\pi\delta_+(\omega)\exp(-i\omega t), \tag{28}$$

$$\int_{t}^{\infty} \exp(-i\omega t')dt' = 2\pi\delta_-(\omega)\exp(-i\omega t), \tag{29}$$

we have

$$W_+(t) = 1 - i\int_{-\infty}^{t} H_1(t')W_+(t')dt', \tag{30}$$

$$W_-(t) = 1 + i\int_{t}^{\infty} H_1(t')W_-(t')dt', \tag{31}$$

which are in agreement with the differential equation and initial conditions for $W_\pm(t)$. The meaning of the integrals in Eqs. (28) and (29) can be made precise by using a limiting process as Lippmann and Schwinger, Ferretti, and Dyson have done. Like all formulas involving the δ_+ function, Eqs. (23) and (24) hold only if the two members of these equations are multiplied by a nonsingular smoothly varying function of ω. We

[6] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, London, 1947).

shall use the term "conditional equality" in referring to this kind of equation.

The temporal development of $\psi_{+\lambda}(t)$ is given by that of $W_+(t)$, namely,

$$\begin{aligned}\psi_{+\lambda}(-\infty)&=\phi_\lambda,\\ \psi_{+\lambda}(0)&=W_+\phi_\lambda=\psi_\lambda,\\ \psi_{+\lambda}(\infty)&=S\phi_\lambda.\end{aligned}\tag{32}$$

Thus, the time-dependence of $\psi_{+\lambda}(t)$ is formally periodic but actually aperiodic, as a result of the singularity of the δ_+ function. Comparison of Eqs. (21), (25), (26), and (30) with the equations given by Schwinger show that $W_+(t)$ satisfies the same equations as the unitary operator which transforms a state vector at the remote past to the state vector at a finite time or the remote future.

The analog of Eq. (18) for the bound state is

$$\psi_s(t)=\exp[i(H_0-E_s)t]\psi_s.\tag{33}$$

It follows from Eqs. (12) and (33) that $\psi_s(t)$ satisfies

$$\psi_s(t)=-i\int_{-\infty}^{t}H_1(t')\psi_s(t')dt',\tag{34}$$

or

$$\psi_s(t)=i\int_{t}^{\infty}H_1(t')\psi_s(t')dt'.\tag{35}$$

Owing to the absence of singularity in Eq. (12), we have

$$\lim_{t\to\pm\infty}\psi_s(t)=0,\tag{36}$$

in agreement with Eqs. (34) and (35).[6a] Note that Eq. (36) is only a conditional equality. The normalization condition

$$(\psi_s(t),\psi_s(t))=1\tag{37}$$

holds even for very large values of t because the two rapidly fluctuating factors in the left-hand side of Eq. (37) cancel each other.

The analogs of Eqs. (14) are

$$\left.\begin{aligned}\psi_s^\dagger(t)W_\pm(t)&=0,\\ W_\pm^\dagger(t)\psi_s(t)&=0.\end{aligned}\right\}\tag{38}$$

These equations may be of interest to the variational treatment of scattering problems.[7]

[6a] Equation (36) is the abbreviated form of the equation

$$\lim_{t\to\pm\infty}(\phi_\mu,\psi_s(t))=0.\tag{36a}$$

The product $(\phi_\mu, \psi_s(t))$ contains the fluctuating factor

$$\exp[i(E_\mu-E_s)t].$$

Thus the same reasoning that has led to the limiting values of $\psi_{\pm\lambda}(t)$ and $W_\pm(t)$ in the above leads to Eq. (36a).

[7] L. Hulthén, Kgl. Fysiograf. Sällskap. Lund. Förh. **14**, No. 21 (1944); B. A. Lippmann and J. Schwinger (see reference 3); M. L. Goldberger, Phys. Rev. **84**, 929 (1951).

The analogs of Eqs. (15), (16), and (17) are

$$\int\psi_{+\lambda}(t)\psi_{+\lambda}^\dagger(t)d\lambda+\sum\psi_s(t)\psi_s^\dagger(t)=1,\tag{39}$$

$$W_+^\dagger(t)W_+(t)=1,\tag{40}$$

$$W_+(t)W_+^\dagger(t)=1-\sum\psi_s(t)\psi_s^\dagger(t).\tag{41}$$

Equation (41) shows that $W_+(t)$ is not a unitary operator when there are bound states present except at $t=\pm\infty$. Thus, the completeness of the eigenvectors ϕ_λ does not imply the completeness of the state vectors $\psi_{+\lambda}(t)$. The state vectors $\psi_s(t)$ should be included in order to obtain a complete orthonormal set.

III. UNITARITY

Let us consider now the connection of the nonunitary operator $W_+(t)$ of the previous section and the unitary operator $U(t, t_0)$ which transforms a state vector $\psi(t_0)$ into the state vector $\psi(t)$. The operator $U(t, t_0)$ is given by any of the following expressions:[8]

$$U(t,t_0)=\exp(iH_0t)\exp[-iH(t-t_0)]\exp(-iH_0t_0),\tag{42}$$

$$U(t,t_0)=\int\psi_{+\lambda}(t)\psi_{+\lambda}^\dagger(t_0)d\lambda+\sum\psi_s(t)\psi_s^\dagger(t_0),\tag{43}$$

or

$$U(t,t_0)=W_+(t)W_+^\dagger(t_0)+\sum\psi_s(t)\psi_s^\dagger(t_0).\tag{44}$$

The summation over the discrete eigenvalues in Eqs. (43) and (44) is essential for U to be unitary. Making t_0 tend to $-\infty$, we obtain a unitary operator $U(t,-\infty)$ which satisfies the equations

$$idU(t,-\infty)/dt=H_1(t)U(t,-\infty),\tag{45}$$

$$\lim_{t\to-\infty}U(t,-\infty)=1,\tag{46}$$

$$U(t,-\infty)=1-i\int_{-\infty}^{t}H_1(t')U(t',-\infty)dt'.\tag{47}$$

We have seen in the previous section that the operator $W_+(t)$ also satisfies these equations. It may seem surprising that there are two different operators that satisfy the same differential equation and initial condition. The explanation is that in deriving the equations satisfied by $W_+(t)$ we have made use of Eq. (25), which is a conditional equality. Indeed, if we use in Eq. (44) the conditional equalities given by Eqs. (25), (26), and (36), we are led to the conclusion that the operators $U(t,-\infty)$ and $W_+(t)$ are identical. The operator $U(\infty,-\infty)$ is then equal to S as usually stated in the literature. It seems to the writer that the mathematical

[8] M. Schoenberg (see reference 3); M. Gell-Mann and F. Low (see reference 4); G. F. Chew and G. C. Wick, Phys. Rev. **85**, 636 (1952); J. Ashkin and G. C. Wick, Phys. Rev. **85**, 686 (1952).

techniques used in the present-day field theories are not sufficient to distinguish between conditional and exact equalities. Thus, the confusion pointed out by Snyder indicates that there is an ambiguity in the determination of the operator U, a question which is of importance in connection with the problem of the bound states.[9, 9a]

The unitarity of the operator $W_+(t)$ at $t=\infty$, i.e., the S-matrix, has been established by Møller and Snyder by means of the time-independent theory of scattering. It can also be derived from the time-dependent theory without much manipulation. It follows immediately from Eq. (40) that

$$S^\dagger S=1. \tag{48}$$

From the equations

$$W_-^\dagger(t)W_-(t)=1, \tag{49}$$

$$W_-^\dagger(t)W_+(t)=S, \tag{50}$$

which can be derived in the same way as Eq. (40), we find

$$W_-(-\infty)=S^\dagger, \tag{51}$$

$$SS^\dagger=1. \tag{52}$$

Thus, S is unitary.

[9] M. Neuman has discussed an additional condition for the unitarity, Phys. Rev. **83**, 671 (1951).

[9a] *Note added in proof.*—We have stated above that the operator $U(t,-\infty)$ is unitary as a result of the unitarity of $U(t,t_0)$ for finite t_0. Dr. M. R. Schafroth has pointed out to the writer that one cannot infer the unitarity of $U(t,-\infty)$ from the unitarity of $U(t,t_0)$ because the unitarity of $U(t,-\infty)$ requires not only

$$\lim_{t_0\to-\infty} U(t,t_0)U^\dagger(t,t_0)=1$$

but also

$$\lim_{t_1,t_2\to-\infty} U(t,t_1)U^\dagger(t,t_2)=1,$$

and there is no reason why the latter should hold. As we have already mentioned above, the operators $U(t,-\infty)$ and $W_+(t)$ are identical if we use the conditional equalities to give $U(t,-\infty)$ a definite limiting value. In this sense the operator $U(t,-\infty)=W_+(t)$ is not unitary, in contrast to $U(t,t_0)$, because of the non-unitarity of $W_+(t)$ which we have shown. Professor W. Pauli has informed the writer that this fact was previously pointed out by Dr. R. Jost in a private discussion. The writer is greatly indebted to Professor Pauli and Dr. Schafroth for these remarks and for their interest in this work.

The product $W_+(t)W_+^\dagger(t)$ satisfies the equation

$$W_+(t)W_+^\dagger(t)=1-i\int_{-\infty}^{t}[H_1(t'),W_+(t')W_+^\dagger(t')]dt'. \tag{53}$$

A unitary $W_+(t)$ would satisfy Eq. (53), but this equation does not imply the unitary of $W_+(t)$.

IV. BORN APPROXIMATIONS

In the above considerations we have not made use of the iteration processes that are usually used in connection with Born's method of successive approximations or Heitler's integral equation. Born's method consists in expanding $W_+(t)$ in the form

$$W_+(t)=1+W_+^{(1)}(t)+W_+^{(2)}(t)+\cdots. \tag{54}$$

The convergence of this series in physical problems has been investigated by Jost and Pais and by Dyson.[10] We shall assume here that we are dealing with a problem in which this series converges. Substituting this power series in Eq. (53) and grouping together terms containing the same power of the coupling constant in the product $W_+(t)W_+^\dagger(t)$, we find

$$\{W_+(t)W_+^\dagger(t)\}^{(0)}=1, \tag{55}$$

$$\{W_+(t)W_+^\dagger(t)\}^{(n)}=-i\int_{-\infty}^{t}[H_1(t'),\{W_+(t')W_+^\dagger(t')\}^{(n-1)}]dt' \quad (n\geqq 1). \tag{56}$$

These equations lead to the result that $W_+(t)W_+^\dagger(t)$ is equal to unity, so that $W_+(t)$ is unitary. This means that the state vectors $\psi_{+\lambda}(t)$ of the free states, when calculated by Born's method, formally form a complete set without the state vectors $\psi_s(t)$.[10a]

The writer is grateful to Dr. T. Y. Wu, Dr. D. Rivier, Dr. J. Pirenne, and Dr. E. Corinaldesi for discussions.

[10] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951); F. J. Dyson, Phys. Rev. **85**, 631 (1952).

[10a] If we apply a similar iteration process to the state vector $\psi_s(t)$ for discrete state and Eq. (34) or (35), $\psi_s(t)$ will turn out to be identically zero. The Born iteration method as described in this section does not, therefore, yield any information concerning the bound states.