Scattering Involving a Bound State*

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Granting that the formation of a bound state is a "sudden" process (as compared to the scattering which may be regarded as a process taking place "adiabatically"), a formulation of the scattering involving a bound state is discussed, in which an independent set of creation-annihilation operators is introduced for a particle in the bound state. There appears here a subsidiary condition which prevents the system from having an unduly increased number of degrees of freedom. In the case of potential scattering, which is studied in this paper, this subsidiary condition restricts the intermediate states in a multiple scattering process to states which are orthogonal to the bound state. This orthogonality condition gives rise to a simple explanation of the theorem concerning the scattering phase shift at zero energy, in which it is stated that when there is one bound state, the scattering phase shift starts with π at zero energy, if it is to go down to zero at extreme high energy.

1. INTRODUCTION

THE formal theory of scattering so far developed is not completely legitimate when there appears a bound state. The shortcomings of the existing theories are rather pressing when we deal with a many-body scattering in which a rearrangement of constituent particles may take place in the exit channel. Although some general ideas were laid down years ago, there are still points to be worked out before they are proved practical. The difficulties inherent in the Lippmann-Schwinger equation have been pointed out and studied by Foldy and Tobocman,[1] Epstein,[2] and Gerjuoy.[3] The problem has been studied also by Ekstein,[4] Haag,[5] and recently by Feshbach[6] from different points of view.

On the other hand, the necessity of revising the current theory has been felt much less urgent in potential scattering and the two-body scattering problem than in the many-body scattering problem. Here it seems that one can do with the same formulation if there appears a bound state as when there is no bound state. But even here several points remain to be studied further. It is known[7] that the scattering phase shift starts with $n\pi$ at zero energy if it goes to zero at extreme high energy, where n is the number of the bound states. This theorem is relevant to the determination of the sign of the scattering length. Speaking of the nucleon-nucleon scattering, the singlet scattering length is negative, while the triplet scattering length is positive. The positive scattering length for the triplet state is expected, because the binding energy of the deuteron is not large, so that the scattering length should behave as if the S-wave phase shift starts with π at zero energy and decreases with increasing energy, which gives rise to the positive scattering length. Though the actual argument should be more complicated because of the tensor force, the gross characteristics of the argument may not be invalidated. In general, we ought to expect a negative scattering length when the potential is attractive, while a positive scattering length is expected when the potential is repulsive. When there is a bound state this argument must be modified in the manner mentioned above. The negative scattering length for an attractive potential is restored when the binding energy of the last bound state is so large that the next bound state is expected if the depth of the attractive potential is increased a little bit.

It is the purpose of this paper to study potential scattering when there is a bound state, with use of a formulation in which creation and annihilation operators for a particle in the bound state are introduced. This formulation is adopted because it can be generalized to apply to a many-body system, and it is then straightforward to discuss the asymptotic conditions in various channels, even if there appear bound particles of different constitution in each one of them. The total Hamiltonian in this formulation is the sum of kinetic energies of stable particles of all sorts and a remainder, which can be termed the effective interaction among them. In order to avoid an undue increase in the number of degrees of freedom of the whole system, some subsidiary condition must be imposed on the state vector of the system. Thus this paper is devoted to the discussion of the simplest case in the theory of scattering under such a subsidiary condition. In Sec. 2, the method of introducing the creation and annihilation operators for the bound state is exhibited.

In Sec. 3 it will be shown that the theorem[7] on the zero-energy phase shift in potential scattering can be derived rather simply when we take into account the subsidiary condition mentioned above. The subsidiary condition designates that only states orthogonal to the bound state are available in the intermediate step of a

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[1] L. L. Foldy and W. Tobocman, Phys. Rev. **105**, 1099 (1957).
[2] S. T. Epstein, Phys. Rev. **106**, 598 (1957).
[3] E. Gerjouy, Phys. Rev. **109**, 1806 (1958).
[4] H. Ekstein, Phys. Rev. **101**, 880 (1956).
[5] R. Haag, Phys. Rev. **112**, 669 (1958); W. Brenig and R. Haag, Fortschr. Physik **7**, 183 (1959).
[6] H. Feshbach, Ann. Phys. **5**, 357 (1958).
[7] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949); P. Swan, Proc. Roy. Soc. (London) **A228**, 10 (1955); J. M. Jauch, Helv. Phys. Acta **30**, 143 (1957); A. Martin, Nuovo cimento **7**, 607 (1958).

scattering process. This orthogonality condition can be represented by introducing some nonlocal force into the Hamiltonian. This nonlocal force gives rise to an "orthogonality phase shift" which starts with π at zero energy and goes down to zero at high energies. The total phase shift is the sum of the "orthogonality phase shift" and the "potential scattering phase shift." The latter is obtained by computing the further distortion of the eigenfunction of the kinetic energy which is caused by the potential.

In Sec. 4 the unitarity of the transformation function and the convergence of the Born series are discussed. The eigenfunctions of the scattering states, together with the bound-state wave function, form a complete set which must be equivalent to the complete set of plane waves. On the basis of this fact, one is led to conjecture that there should be some unitary transformation which transforms one set into the other. However, we have not yet succeeded in establishing this point. On the other hand, we can pin down the source of the difficulty. It is correlated with the nominal origin of the bound state which is to be discovered among the unperturbed waves. The eigenstate of the kinetic energy under the subsidiary condition must be defined by taking the limit of the matrix element of some unitary transformation function in a certain way, and the convergence to the limit is not uniform at zero energy. The zero energy is the nominal origin of the bound state, and it must be treated very carefully. The clarification of this point is left for future work.

In order to supplement the discussions in the text, the orthogonality of the bound state to the scattering state is considered in Appendix I in the ordinary formulation of the scattering theory.

2. INTRODUCTION OF CREATION-ANNIHILATION OPERATORS FOR A BOUND STATE

We shall exhibit here a method which is useful in dealing with a particle in a bound state. The exposition is given fully in order to provide for treatment of a many-body system in further publications, although it is possible to shorten it substantially so long as we restrict ourselves to the potential scattering. The legitimacy of the following method as used in potential scattering is established through the two facts which are to be proved in Secs. 3 and 4. The first is that the formation of a bound state, which takes place as the attractive potential becomes deep enough, is a sudden change so that the notion of an adiabatic change of the system is inapplicable to the bound state; consequently, it makes sense to regard the particle in the bound state as an independent entity, when we start discussing the scattering process, to which the notion of an adiabatic change is applicable in some way or other. The second is that in our formulation there appears a subsidiary condition besides the Hamiltonian, which causes some complication as compared to the current theory; however, it is rewarding to work with this slightly more complicated formulation, because the subsidiary condition actually helps us to understand a feature of the system, namely, the scattering phase shift at zero energy.

We consider bosons of S-wave state in an external potential,[8] as the first step of treating bound states in a more general case. The commutation relation for the creation and annihilation operators for bosons in the spherical S-wave state is the usual one,

$$[a_{k'},a_k^\dagger]=\delta(k'-k). \tag{2.1}$$

The Hamiltonian to be dealt with can be written in the form,[9]

$$H=\int dk\, W_k a_k^\dagger a_k+\int\int dkdk'(k|V|k')a_k^\dagger a_{k'}, \tag{2.2}$$

where W_k is the kinetic energy of a boson with the wave number k. We introduce the matrix notation for the kinetic energy and rewrite the Hamiltonian (2.2) in the form

$$H=\int\int dkdk'(k|W+V|k')a_k^\dagger a_{k'}. \tag{2.2'}$$

Hereafter we assume that there is only one bound state. Our method of treating a bound state, generally speaking, consists of the following two steps:

(i) *Introduction of redundant variables.*—We introduce a set of creation and annihilation operators, which satisfy the commutation relation

$$[b,b^\dagger]=1. \tag{2.3}$$

b and $b^\dagger$ are redundant variables at the outset, although the operator $b^\dagger b$ will describe the number of particle in the bound state later on. We are going to extend the Hilbert space so as to include state vectors of the b operators as well as those of the a operators. To keep the modified Hilbert space as a whole equivalent to the original one, we impose the subsidiary condition

$$b^\dagger b\Psi=0 \tag{2.4}$$

on the extended state vector, which we denote by Ψ. It is evident at this stage that the whole problem remains equivalent to the original one.

(ii) *Interchange of the redundant mode with a physically meaningful wave packet.*—Let us call a particle described in terms of the a operators an a particle. Also a particle in the bound state is called a b particle. We perform

[8] We avoid a potential of long range like the Coulomb force; in such a case of infinitely many bound states will be formed once the potential is switched on.

[9] If we take the model more seriously, there should be a pair creation and annihilation term to be added to (2.2); these are obtained by replacing $a_k^\dagger a_{k'}$ in the potential by $\frac{1}{2}(a_k^\dagger a_{k'}^\dagger+a_{k'}a_k)$. Since this does not affect the essential points of the following argument, we can start from the Hamiltonian (2.2). We can suppose that the pairs are already eliminated by means of a canonical transformation.

then a canonical transformation by which the redundant particle is replaced by some wave packet for an a particle. The subsidiary condition must be transformed at the same time. *The transformation is uniquely defined when we require that the subsidiary condition does not involve a* b *operator after the transformation and represents a reduction in the degree of freedom of the* a *particles.* The transformed subsidiary condition actually designates that only states of a particles orthogonal to the wave packet are permissible after the transformation.

Now let us study the transformation stated above in detail and apply it specifically to the Hamiltonian (2.2). We denote the normalized weight function for the wave packet by $f(k)$. First it is in order to define the operator for the number of particles with this wave packet. This is defined as

$$N[f]=\int dk\, a_k^\dagger f(k)\int dk'\, a_{k'}f^*(k'). \tag{2.5}$$

Let us then consider the operator

$$R=\lambda b^\dagger\int dk\, a_k f^*(k), \tag{2.6}$$

where λ is an arbitrary constant. In the state $R\Psi$ which is the transform of Ψ by means of R, the number of a particles with wave function $f(k)$ is decreased by one, while the number of b particles is increased by one as compared to the situation represented by Ψ. Thus R is the operator which replaces a wave packet $f(k)$ by a corresponding b particle. If we multiply Ψ by a suitable function of the operator R, a particles with wave function $f(k)$ originally existing in Ψ will be replaced by b particles. In making a choice of such a function we remind ourselves that we are going to achieve the desired result by means of a unitary transformation in order to leave the relationship of Hermitian conjugates invariant among operators and to avoid unnecessary complication in the results. Accordingly we are led to try a unitary transformation generated by the Hermitian operator, $R+R^\dagger$; the transformation function which we consider is

$$U=\exp[i(R+R^\dagger)]. \tag{2.7}$$

The condition that the transformed subsidiary condition does not involve b operators determines the parameter λ, and we obtain the desired new state vector

$$\Psi'=U^{-1}\Psi,$$

which is to be used in the discussion of a scattering process. By virtue of the form of the new subsidiary condition, we can speak of a b particle quite freely in the new representation, as an entity independent of a particles. After some manipulations, we have

$$U^{-1}bU=(\cos\lambda)b+i\sin\lambda\int dk\, f^*(k)a_k. \tag{2.8}$$

By setting

$$\lambda=\pi/2, \tag{2.9}$$

we obtain the new subsidiary condition of the desired form:

$$U^{-1}b^\dagger bU\cdot\Psi'=N[f]\cdot\Psi'=0. \tag{2.10}$$

The transformed a operators are given, then, by

$$U^{-1}a_kU=a_k-f(k)\left\{\int dk'\, f^*(k')a_{k'}-ib\right\}, \tag{2.11}$$

and its Hermitian conjugate. By substitution of (2.11) and its Hermitian conjugate into the original Hamiltonian (2.2′), the new Hamiltonian is given as

$$H=H_a+H_b+H_{a-b}, \tag{2.12}$$

$$H_a\equiv\int\int dkdk'\, a_k^\dagger(k|W+V|k')a_{k'}+\bar{E}N[f]$$
$$-\left\{\int\int dkdk'\, a_k^\dagger(k|W+V|k')f(k')\times\int a_{k''}f^*(k'')dk''+\text{Herm. conj.}\right\}, \tag{2.12′}$$

$$H_b\equiv\bar{E}b^\dagger b, \tag{2.12″}$$

$$H_{a-b}\equiv\int\int dkdk'\, a_k^\dagger(k|W+V-\bar{E}|k')f(k')\cdot b+\text{Herm. conj.}, \tag{2.12‴}$$

where $\bar{E}$ is the energy averaged over the wave packet $f(k)$,

$$\bar{E}=\int\int dkdk'\, f^*(k)(k|W+V|k')f(k'); \tag{2.13}$$

H_a and H_b involve, respectively, only a operators and b operators, while H_{a-b} represents the interaction between an a particle and a b particle. By inspection of (2.12‴) we recognize that H_{a-b} vanishes when $f(k)$ is an eigenfunction of the total Hamiltonian. Since $f(k)$ must be normalizable, it must be a bound-state eigenfunction. When $f(k)$ is the bound-state eigenfunction, $\bar{E}$ is equal to the exact eigenvalue E of the bound state, and the Hamiltonian reduces to the form

$$H=H_a^0+H_b, \tag{2.14}$$

$$H_a^0\equiv\int\int dkdk'\, a_k^\dagger(k|W+V|k')a_{k'}-EN[f]. \tag{2.14′}$$

Our next task is to compute a complete set of eigenfunctions of H_a^0 under the subsidiary condition (2.10), and then to derive the scattering cross section. These problems will be discussed in the following sections. A brief comment on the nature of that problem is proper here. We introduce projection operators $\Lambda_{\parallel}$ and $\Lambda_{\perp}$

defined as matrices with matrix elements, respectively, given by

$$(k'|\Lambda_{\parallel}|k)=f(k')f^*(k), \tag{2.15}$$

$$(k'|\Lambda_{\perp}|k)=(k'|1-\Lambda_{\parallel}|k)=\delta(k-k')-f(k')f^*(k). \tag{2.15'}$$

H_a^0 can be written then in the form

$$H_a^0=\int\int dkdk'\, a_k^\dagger(k|\Lambda_{\perp}(W+V)\Lambda_{\perp}|k')a_{k'}. \tag{2.16}$$

It is clear now that the problem to be solved is almost the same as the original one in which the Hamiltonian is given by (2.2), but there is a difference in that it must be solved under the constraint (2.10). It is clear that the subsidiary condition is compatible with the Hamiltonian (2.16), as it should be.

As remarked earlier, the desired result can be achieved much more easily in the case of potential scattering than by the method above. One can make the following canonical transformation

$$a_k=c_k-if(k)b, \tag{2.17}$$

and its Hermitian conjugate, where c_k and $c_k^\dagger$ are concerned with waves orthogonal to $f(k)$ only:

$$\int c_k f^*(k)dk=0, \tag{2.18}$$

and satisfy instead of (2.1) the commutation relation

$$[c_{k'},c_k^\dagger]=(k'|\Lambda_{\perp}|k). \tag{2.19}$$

If one substitutes (2.17) into the original Hamiltonian (2.2) one obtains an operator corresponding to (2.16),

$$H_c^0=\int\int dkdk'\, c_k^\dagger(k|W+V|k')c_{k'}, \tag{2.20}$$

which, however, is not accompanied by any subsidiary condition. It is readily seen that the solution of the problem under the subsidiary condition (2.10) is equivalent to the determination of the eigenfunctions of the Hamiltonian (2.20) in which the modified commutation relation (2.19) must be used. In a more general case of a many-body problem, the required transformation is not a linear relation as given by (2.17), and it is more difficult to find than in the case of potential scattering. In such a case it is really helpful to proceed along the line described in this section.

3. ORTHONORMAL EIGENFUNCTIONS OF THE KINETIC ENERGY UNDER THE ORTHOGONALITY CONDITION

Let us study the orthonormal set of eigenfunctions of the kinetic energy, under the orthogonality condition which we denote by $K_{\perp}$,

$$K_{\perp}\equiv\int\int dkdk'\, a_k^\dagger(k|\Lambda_{\perp}W\Lambda_{\perp}|k')a_{k'}. \tag{3.1}$$

The effect of the potential in our Hamiltonian (2.16) will be considered in the next section. The corresponding Schrödinger equation in momentum space is given by

$$W_{k'}h(k'k)+\int dk''(k'|(\bar{W}-W_{k'})\Lambda_{\parallel}+\Lambda_{\parallel}W_{k''}|k'')h(k''k)=W_k h(k',k), \tag{3.2}$$

where we have put

$$\bar{W}=\int dk|f(k)|^2W_k.$$

Since the orthogonality of $h(k'k)$ to $f(k')$ is easily established when W_k does not vanish, (3.2) reduces into

$$(W_{k'}-W_k)h(k'k)=f(k')\int dk''\, f^*(k'')W_{k''}h(k''k). \tag{3.3}$$

We can show it is sufficient to consider the solution of Eq. (3.3) under the standing wave boundary condition. Then, disregarding the normalization, we can put $h(k'k)$ into the form

$$h(k'k)=\delta(k'-k)+P\frac{1}{W_{k'}-W_k}f(k')X(k). \tag{3.4}$$

By making use of the orthogonality of $h(k'k)$ to $f(k')$ again, the indeterminate $X(k)$ in (3.4) is given by

$$X(k)=f^*(k)/J(k), \tag{3.5}$$

where we have put

$$J(k)\equiv\int dk'\, P\frac{1}{W_{k'}-W_k}|f(k')|^2=\frac{1}{W_k}\left(\int dk'\, P\frac{1}{W_{k'}-W_k}W_{k'}|f(k')|^2-1\right). \tag{3.6}$$

With use of the last statement in (3.6) for $J(k)$, it is straightforward to verify that the solution given by (3.4)–(3.6) actually satisfies Eq. (3.3), hence Eq. (3.2).

$h(k'k)$ does not represent a free S wave any more, but a distorted wave. Let us then calculate the phase shift due to the orthogonality, which we denote by $\delta_0(k)$, as a function of the wave number k associated with the energy W_k of the system. It is determined by the equation

$$\tan\delta_0(k)=-\pi f(k)X(k)\left(\frac{\partial W_k}{\partial k}\right)^{-1}=-(\pi|f(k)|^2)\Big/\left(J(k)\frac{\partial W}{\partial k}\right), \tag{3.7}$$

since we are dealing with a solution under the standing

wave boundary condition.[10] We note there that we have at $k=0$

$$\left(|f(k)|^2\Big/\frac{\partial W_k}{\partial k}\right)\Big|_{k=0}=0, \tag{3.8}$$

since $f(k)$ is k times the Fourier transform of a function in configuration space which is normalizable,[11] and $(\partial W_k/\partial k)$ is a function which is linear in k in the non-relativistic mechanics. We also have

$$|f(\infty)|^2=0, \tag{3.9}$$

since $|f(k)|^2$ must be integrable. We define $\delta_0(\infty)$ by

$$\delta_0(\infty)=0, \tag{3.10}$$

since we have[12]

$$\tan\delta_0(\infty)=0, \tag{3.10'}$$

as a result of (3.9).

As is seen by the inspection of the integrand in (3.6), the sign of the real function $J(k)$ of k is positive for very small k, while it is negative for a very large k. $J(k)$ must be a continuous function of k, consequently the total number of its zeros is an odd number. We label these zeros by an index and arrange them in the order of their magnitudes,

$$k_1<k_2<\cdots<k_{2n+1}.$$

Then the sign of $J(k)$ in each interval is determined as

$$\begin{aligned} &J(k)<0, \quad \text{when } k_{2n+1}<k,\\ &\qquad k_{2m+1}<k<k_{2m+2} \quad (m=0,1,\cdots,n-1),\\ &J(k)>0, \quad \text{when } k<k_1,\\ &\qquad k_{2m}<k<k_{2m+1} \quad (m=1,2,\cdots,n). \end{aligned} \tag{3.11}$$

Noting that $|f(k)|^2$ is non-negative, and excluding the accidental degeneracy such as has been pointed out by Martin,[13] we can then conclude from (3.7), (3.10), and (3.11), that $\delta_0(k)$ in each interval must be restricted within the limit given by

$$\begin{aligned} &\pi/2>\delta_0(k)\geq 0 \quad &&\text{when } J(k)<0,\\ &\pi\geq\delta_0(k)>\pi/2 \quad &&\text{when } J(k)>0,\\ &&&\text{in particular } k<k_1. \end{aligned} \tag{3.12}$$

Finally, remembering (3.8), we conclude that

$$\delta_0(0)=\pi. \tag{3.13}$$

This establishes that the orthogonality phase shift $\delta_0(k)$ takes care of the discontinuity of the phase shift at zero energy which takes place when there appears a new bound state.

The normalization of $h(k',k)$ is given by multiplying the solution in (3.4) by $\cos\delta_0(k)$. Letting the same notation denote the normalized solution in this case, we have

$$h(k'k)=\delta(k-k')\frac{\mathrm{Re}\,\Phi(k)}{|\Phi(k)|}-P\frac{1}{W_k-W_{k'}}\frac{f(k')f^*(k)}{|\Phi(k)|}, \tag{3.14}$$

where we have put

$$\begin{aligned}\Phi(k)&=-J(k)+i\pi|f(k)|^2(\partial W_k/\partial_k)^{-1}\\ &=\int dk'|f(k')|^2\left(P\frac{1}{W_k-W_{k'}}+i\pi\delta(W_k-W_{k'})\right).\end{aligned} \tag{3.15}$$

We can readily establish the orthogonality among $h(k'k)$'s with different k,

$$\int h^\dagger(k'k'')h(k''k)dk''=\delta(k'-k), \quad (W_kW_{k'}\neq 0) \tag{3.16}$$

in which use has been made of the rule for dealing with singular functions,

$$\begin{aligned}&P\frac{1}{W-W''}P\frac{1}{W''-W'}\\ &\qquad=P\frac{1}{W-W'}\left(P\frac{1}{W-W''}+P\frac{1}{W''-W'}\right)\\ &\qquad\quad-\pi^2\delta(W-W'')\delta(W'-W''),\\ &P\frac{1}{W-W''}\delta(W''-W')=P\frac{1}{W-W'}\delta(W''-W').\end{aligned} \tag{3.17}$$

As for the completeness proof, we must be more careful. Here we have to notice that the wave function of the bound state $f(k)$ is itself an eigenfunction of the Schrödinger Eq. (3.2) for the eigenvalue $W_k=0$. We should have

$$\int_{+0}^{\infty}dk''\,h(k'k'')h^\dagger(k''k)=(k'|\Lambda_\perp|k). \tag{3.18}$$

[10] The treatment of S wave is made here in almost the same way as has been done by Kohn. See, W. Kohn, Phys. Rev. 84, 495 (1951); especially, see Sec. II of his paper for the detail of the derivation of Eq. (3.7).

[11] Explicitly, $f(k)$ is given by

$$f(k)=(2/\pi)^{\frac{1}{2}}\int_0^\infty \sin kr\, u(r)dr,$$

where $\varphi(r)=u(r)/r$ is the wave function of the bound state in configuration space in ordinary sense. In our treatment of momentum space, the degree of freedom r (and hence k) is treated in a one-dimensional space [or, the volume element is dr (dk), instead of r^2dr (k^2dk)], and the Fourier transform is made only into sine functions because of the boundary condition at $r=0$.

[12] Since only $\exp[2i\delta(k)]$ is meaningful as the ratio of the outgoing amplitude to the ingoing amplitude, there is an arbitrariness in the definition of the phase shift by a multiple of π. This arbitrariness is settled by (3.10), the *difference* between phase shifts at different energies being a well-defined quantity. The last point is proved by Levinson and Swan, reference 7. The continuity of the phase shift as a function of k is made use of in the arguments which lead into Eq. (3.13).

[13] See reference 7. In such a case of accidental degeneracy, there appears a state with positive energy which looks like a bound state, and we must have one more orthogonality condition which gives rise to $\delta(0)-\delta(\infty)=2\pi$.

However, we have not yet succeeded in establishing (3.18) directly with use of $h(kk')$ given in (3.14). The lower limit of integration in (3.18) is denoted by $+0$ in order to emphasize that the point $k''=0$ is excluded. If the point $k''=0$ were a regular point of the integrand it would not make any difference whether it is explicitly included or excluded in the domain of integration. Actually the point $k''=0$ must be some kind of singularity of $h(k'k'')$. In this connection it is to be noted that $h(k'k)$ is given by taking the limit $\lambda\to 1$ of the matrix element of a certain unitary transformation function, which transforms eigenfunctions of the unperturbed Hamiltonian into eigenfunctions of the Hamiltonian

$$K^{(\lambda)}=\int\int dkdk'\, a_k^\dagger \times(k|(1-\lambda\Lambda_{11})W(1-\lambda\Lambda_{11})|k')a_{k'}. \quad (3.19)$$

Apparently, in the case $\lambda=0$ the eigenfunctions of the corresponding Schrödinger equation are unperturbed spherical waves, while in the case $\lambda=1$ they are expected to coincide with what we have obtained in (3.14). Further detail of the discussion of the eigenfunction of the Hamiltonian (3.19), as a function of λ as well as of the wave number, is given in Appendix II. The conclusion there obtained is that we can define the energy $W_b(\lambda)$ such as, when the energy of the system is larger than $W_b(\lambda)$, the eigenfunction $h^{(\lambda)}(k'k)$ associated with the Hamiltonian (3.19) converges uniformly to its limit $h(k'k)$ as we let λ approach unity. $W_b(\lambda)$ itself, however, approaches zero as we take the limit $\lambda\to 1$.

4. CONSTRUCTION OF THE S MATRIX. CONCLUDING REMARKS

We have not been able to show explicitly how the bound-state wave function $f(k)$ is peeled off from the lower end of the spectrum $W_b(\lambda)>W_k>0$ of the unperturbed waves (along the line remarked at the end of the last section), when we take the limit $\lambda\to 1$. However, it may be reasonable to make a conjecture that there exists a unitary transformation T_0 which transforms the creation-annihilation operators according to

$$T_0^\dagger a_k T_0=\int h(kk')a_{k'}dk'+f(k)a_0, \quad (4.1)$$

and its Hermitian conjugate. Here $a_0^\dagger$ and a_0 mean the creation and annihilation operator, respectively, of a normalizable wave packet concentrated at zero energy.

Reminding ourselves of the situation at the end of Sec. 2, we summarize the subsidiary condition and the Hamiltonian at this stage. The subsidiary condition takes the form

$$a_0^\dagger a_0\Psi''=0, \quad (\Psi''=T_0^\dagger\Psi'). \quad (4.2)$$

This means that the subsidiary condition is now of negligible importance since a single point at the end of the continuous spectrum may be either included or omitted in the domain of integration, if the integrand is regular at zero energy (as is usually the case if there is no second bound state). The Hamiltonian thus takes the form

$$T_0^\dagger\left\{\int\int dkdk'\, a_k^\dagger(k|\Lambda_\perp(W+V)\Lambda_\perp|k')a_{k'}+Eb^\dagger b\right\}T_0 = \int W_k a_k^\dagger a_k dk+Eb^\dagger b +\int\int dkdk'(k|\bar V|k')a_k^\dagger a_{k'}, \quad (4.3)$$

where we have put

$$(k|\bar V|k')=\int\int dk''dk'''\, h^\dagger(kk'')(k''|V|k''')h(k'''k'). \quad (4.4)$$

The effective potential $\bar V$ will be discussed below. In (4.3), the creation-annihilation operators, $a_k^\dagger$ and a_k, refer to the particle in an eigenstate of $K_\perp$, (3.1), described in terms of the wave function $h(k'k)$.

Now, the last step in our discussion of the scattering is to diagonalize the Hamiltonian (4.3), which may be achieved by applying the current theory of scattering to the following Hamiltonian:

$$H_{\text{pot. scat.}}=\int a_k^\dagger a_k W_k dk+\int\int dkdk'(k|\bar V|k')a_k^\dagger a_{k'}; \quad (4.3')$$

the remainder of the Hamiltonian (4.3), pertaining to the b particle, is irrelevant to the following discussion. The deviation of the effective potential $\bar V$ from the original potential V is caused by the orthogonality of the relevant states to the bound state, and is expected to become negligible when the energy of the incoming particle becomes much larger than the binding energy of the bound state; or, in equation, we expect to have

$$(k|\bar V|k')\approx(k|V|k'), \quad \text{when } W_k, W_{k'}\gg E. \quad (4.5)$$

This point has been confirmed by calculating $(k|\bar V|k')$ in a number of examples. One example is the square well (local) potential, and another example is the nonlocal potential of the simple form defined by

$$(k|V|k')=-b^2\frac{k}{M^2+k^2}\frac{k'}{M^2+k'^2},$$

where b and M are parameters which determine the strength and the range of the potential, respectively.

In order to go farther with mathematical rigor, we need to know a condition on the form of potentials under which the Born series for the phase shift converges. Then we must show that $(k|\bar{V}|k')$ satisfies the required condition. Since that condition is not known in its most general form, we have to be satisfied only with making a conjecture which is based on facts verified in examples. Our conjecture is that we can apply Born approximations in the discussion of the effect of the effective potential $\bar{V}$, when the binding energy of the bound state is rather small so that the second bound state is far from being expected. In other words, it is conjectured that we can apply the formal theory of scattering without any modification to the Hamiltonian $H_{\text{pot. scat.}}$, (4.3′). The corresponding phase shift $\delta_P(k)$ starts with zero at zero energy, if it goes down to zero at high energies. The total phase shift is given by the sum of the "orthogonality phase shift" and the "potential scattering phase shift."

As for the formal proof of the statement made above for the construction of the total phase shift, there exists a unitary transformation function T_P, which diagonalizes the Hamiltonian (4.3′):

$$T_P^{\dagger}\left\{\int a_k^{\dagger}a_k W_k dk+\int\int dkdk'(k|\bar{V}|k')a_k^{\dagger}a_{k'}\right\}T_P = \int a_k^{\dagger}a_k W_k dk, \quad (4.6)$$

and which keeps the subsidiary condition (4.2) invariant, since the operators a_0 and $a_0^{\dagger}$ do not appear in (4.3′). The structure of the transformation function is such that

$$T_P=\exp\left\{\int\int dkdk'\, a_k^{\dagger}a_{k'}P\frac{1}{W_k-W_{k'}}(k|F|k')\right\}, \quad (4.7)$$

and the phase shift $\delta_P(k)$ is given in terms of the diagonal element of the operator F,[14]

$$\delta_P(k)=\pi(\partial W/\partial k)^{-1}(k|F|k). \quad (4.8)$$

The transformation function T_0 should have a similar structure when we deal with the case $\lambda\neq 1$ before we take the limit $\lambda\to 1$, as is discussed at the end of the last section and in Appendix II. We conjecture the structure of the exponent is left essentially unchanged while the limit $\lambda\to 1$ is being taken, if we deal with the matrix element pertaining to the states with energy larger than $W_b(\lambda)$. This furnishes us with the formal proof of the additivity of the two phase shifts, δ_0 and δ_P, when we define the S matrix according to[14]

$$\begin{aligned}S=&\lim_{\substack{t_2\to+\infty\\ t_1\to-\infty}}\exp\left[it_2\int dk\, a_k^{\dagger}a_k W_k\right]\\ &\times\exp\left[i(t_1-t_2)\int dkdk'\, a_k^{\dagger}a_{k'}(k|\Lambda_1(W+V)\Lambda_1)k'\right]\\ &\times\exp\left[-it_1\int dk\, a_k^{\dagger}a_k W_k\right]\\ =&\lim_{\substack{t_2\to+\infty\\ t_1\to-\infty}}\exp\left[it_2\int dk\, a_k^{\dagger}a_k W_k\right]T_0T_P\\ &\times\exp\left[i(t_1-t_2)\int dk\, a_k^{\dagger}a_k W_k\right]T_P^{-1}T_0^{-1}\\ &\times\exp\left[-it_1\int dk\, a_k^{\dagger}a_k W_k\right]\\ =&\exp\left[i\int\delta_0(k)a_k^{\dagger}a_k dk\right]\exp\left[i\int\delta_P(k)a_k^{\dagger}a_k dk\right]\\ &\times\exp\left[i\int\delta_P(k)a_k^{\dagger}a_k dk\right]\exp\left[i\int\delta_0(k)a_k^{\dagger}a_k dk\right]\\ =&\exp\left[2i\int(\delta_0(k)+\delta_P(k))a_k^{\dagger}a_k dk\right]. \quad (4.9)\end{aligned}$$

Here we have dropped the part of the Hamiltonian pertaining to b particles, because it is irrelevant to the present discussion.

In our formulation of scattering involving a bound state, only states which are orthogonal to the bound state are available for the intermediate states of a multiple scattering process. The discussion on this point is supplemented in Appendix I, where the orthogonality condition is treated for the Lippmann-Schwinger equation.

Summarizing, we have shown that the characteristic jump of the phase shift by π at zero energy, which takes place when there appears a bound state, can be taken into account if we explicitly make use of the condition that scattering states are orthogonal to the bound state. There remain, however, some mathematical points to be worked out, namely (i) the structure of the transformation function T_0 as the limit $\lambda\to 1$ is taken, and (ii) the convergence proof, or the proof of the possibility of analytical continuation as a function of the potential depth for the Born series as used in the construction of T_P. Nonetheless, the physical situation seems to have been clarified. The orthogonality condition is equivalent to the introduction of a nonlocal potential which distorts the eigenfunction of the kinetic energy and replacing the potential V by $\bar{V}$. The effect

[14] S. Tani, Phys. Rev. **115**, 711 (1959).

of the orthogonality condition becomes small when the energy of the incident particle is very large as compared to the binding energy. Thus the Born approximations are relatively reliable at high energies.[15]

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APPENDIX I. SCATTERING PROCESSES UNDER THE ORTHOGONALITY CONDITION

Usually a discussion of a scattering process proceeds without any projection operator such as the $\Lambda_\perp$ as appearing in Eq. (2.16). Let us now consider how essential it is to have the projection operator $\Lambda_\perp$ in the Hamiltonian H_a^0 (2.16). In addition, through the discussion of multiple scattering, we shall obtain a picture of the part assigned to the bound state in the course of a scattering process.

Let us begin with examining the ordinary Schrödinger equation in momentum space:

$$W_{k'}\varphi(k'k)+\int dk''(k'|V|k'')\varphi(k''k)=W_k\varphi(k'k), \quad \text{(A.1)}$$

where there is no projection operator and W_k is non-vanishing. As usual we try to find a solution of (A.1) by putting the wave function in the form

$$\varphi(k'k)=\delta(k'-k)+\chi(k'k). \quad \text{(A.2)}$$

The function $\chi(k'k)$ must satisfy the equation

$$(W_{k'}-W_k)\chi(k'k)+\int dk''(k'|V|k'')\chi(k''k)+(k'|V|k)=0. \quad \text{(A.3)}$$

If we project Eq. (A.3) onto $f(k)$ to the left-hand side, we have

$$(E-W_k)\left[f^*(k)+\int dk' f^*(k')\chi(k''k)\right]=0, \quad \text{(A.4)}$$

from which we must conclude that

$$\int f^*(k')\chi(k'k)dk'=-f^*(k). \quad \text{(A.5)}$$

Thus the component of χ parallel to $f(k)$ is given, once and for all, by

$$\chi_{\parallel}(k'k)=-f(k')\cdot f^*(k). \quad \text{(A.6)}$$

On the other hand, the equation to be satisfied by the component of χ orthogonal to $f(k)$ is

$$\int dk''(k'|\Lambda_\perp W\Lambda_\perp-W_k\Lambda_\perp|k'')\chi(k''k)+\int dk''(k'|\Lambda_\perp V\Lambda_\perp|k'')\chi(k''k)+(k'|\Lambda_\perp V|k)=0. \quad \text{(A.7)}$$

Here we need the eigenfunctions of the kinetic energy under the condition of orthogonality to $f(k)$:

$$K_\perp=\int\int dkdk'\, a_k^\dagger a_{k'}(k|\Lambda_\perp W\Lambda_\perp|k'). \quad \text{(A.8)}$$

As was shown in Sec. 3, for all nonvanishing W_k, there is a "normalized" (in a sense similar to plane waves) solution of the equation

$$\int dk''(k'|\Lambda_\perp W\Lambda_\perp|k'')h(k''k)=W_k h(k'k), \qquad \int dk'' h^\dagger(kk'')(k''|\Lambda_\perp W\Lambda_\perp|k)=W_k h^\dagger(k_1k'). \quad \text{(A.9)}$$

In terms of h and $h^\dagger$, we can define the Green function associated with the Schrödinger Eq. (A.9). It has the matrix element

$$(k'|G(W_k)|k'')=\int dl\, h(k'l)P\frac{1}{W_l-W_k}h^\dagger(lk'')-\frac{1}{W_k}f(k')f^*(k''), \quad \text{(A.10)}$$

in the spherical S-wave representation. With use of $G(W_k)$, the solution of (A.7) is given by

$$\chi_\perp(k'k)=(k'|G(W_k)\Lambda_\perp V|k)+(k'|G(W_k)\Lambda_\perp V\Lambda G(W_k)\Lambda_\perp V|k)+\cdots. \quad \text{(A.11)}$$

Hence the solution of the original Schrödinger equation is given by

$$\varphi(k'k)=\delta(k'-k)+\chi_\perp(k'k)-f(k')f^*(k). \quad \text{(A.12)}$$

From Eqs. (A.12) and (A.11), we are led to the following picture of the scattering processes. When the initial spherical S wave strikes the potential, only that part of the emerging wave which is orthogonal to the bound state is transmitted to the wave zone, while the remainder is trapped by the scattering center and forms the bound state. The total wave undergoes the effect of the potential repeatedly, and in each of the multiple scattering processes only waves orthogonal to the bound state are transmitted to the wave zone, while leaving at each step some contribution to the amplitude of the bound state. It is to be noted that $G(W_k)$ is

[15] See for instance, C. Zemach and A. Klein, Nuovo cimento **10**, 1078 (1958).

commutable with the projection operator $\Lambda_\perp$

$$\Lambda_\perp G(W_k)=G(W_k)\Lambda_\perp=\Lambda_\perp G(W_k)\Lambda_\perp, \qquad (A.13)$$

so that no projection operator $\Lambda_{||}$ can appear in the middle of a sequence of operator $G(W_k)\Lambda_\perp V\Lambda_\perp$ in (A.11). This means that the bound state, if once formed, does not affect the subsequent stages of a multiple scattering. The total amplitude of the bound state generated in the course of a multiple scattering is exactly what is necessary to make the whole solution orthogonal to the bound state. It is also to be noted this amplitude is given by (A.6) *without recourse to Born expansion.*

APPENDIX II. THE LIMITING PROCESS $\lambda \to 1$ INTRODUCED IN 3

Let us study the eigenfunction of the Hamiltonian $K^{(\lambda)}$ introduced in (3.19) of the text,

$$K^{(\lambda)}=\int\int dkdk'\, a_k^\dagger(k|\,(1-\lambda\Lambda_{||})W(1-\lambda\Lambda_{||})\,|k')a_{k'}, \qquad (B.1)$$

as a function of both λ and the wave number. The normalized solution of the Schrödinger equation is given by

$$h^{(\lambda)}(k'k')=\left\{\delta(k'-k)-P\frac{1}{W_{k'}-W_k}\lambda f(k')f^*(k)\right.$$
$$\left.\times\frac{W_k+(1-\lambda)W_{k'}}{-\lambda(2-\lambda)W_kJ(k)+(1-\lambda)^2}\right\}\cos\delta^{(\lambda)}(k), \qquad (B.2)$$

where the relevant phase shift is given by

$$\tan\delta^{(\lambda)}(k)=\frac{\pi}{(\partial W/\partial k)}\frac{\lambda(2-\lambda)\,|f(k)|^2}{-\lambda(2-\lambda)J(k)+(1-\lambda)^2/W_k}. \qquad (B.3)$$

From the inspection of (B.3) we see that, if we are going to take the limit, $\lambda\to 1$ and $k\to 0$, the convergence to the limit is not uniform. In general, as λ increases from zero there appears a point where the maximum of the phase shift reaches $\pi/2$. Let us denote that energy by W_c and the corresponding value of λ by λ_c. With λ larger than λ_c, there are two points on both sides of W_c where $\delta^{(\lambda)}(k)$ takes the value $\pi/2$. The maximum of the phase shift, which is reached somewhere between these two points, does not exceed π, but approaches it as λ approaches unity. If the form of $f(k)$ is complicated as a function of k, it might happen that $J(k)$ is sufficiently complicated that a few more pairs of points appear at which $\delta^{(\lambda)}$ assumes the value $\pi/2$; however, what is essential in the following is the fact that the point appearing at the lowest energy, which we dnote by W_r, approaches zero as λ approaches unity. When λ is almost equal to unity, W_r is given by

$$W_r\sim\frac{(1-\lambda)^2}{\lambda(2-\lambda)}\frac{1}{J(0)}, \quad \text{when } \lambda\sim 1. \qquad (B.4)$$

On the other hand, the phase shift at zero energy, $\delta^{(\lambda)}(0)$, keeps the value zero if λ is not equal to unity.

Now we define the limit by taking the limit $\lambda\to 1$ first and taking the limit $k\to 0$ afterward. In order to get the same results as obtained earlier, (3.4–7), we adopt the following prescription for taking the limit. First, consider the phase shift at the energy W_b (the suffix b here represents the "boundary"),

$$W_b(\lambda)=\frac{1-\lambda}{\lambda(2-\lambda)}\frac{1}{J(0)}\sim\frac{W_r}{1-\lambda}. \qquad (B.5)$$

By substituting (B.5) into (B.3), we can see that the phase shift at W_b is almost π when λ is almost equal to unity. One can readily see in (B.2) that for an energy larger than W_b the limit $\lambda\to 1$ converges uniformly and we have

$$h(k'k)=\lim_{\lambda\to 1}h^{(\lambda)}(k'k), \quad \text{when } W_k>W_b(\lambda). \qquad (B.6)$$

For energy smaller than W_b, the corresponding limit $\lambda\to 1$ of $h^{(\lambda)}(k'k)$ should give $f(k')$ when it is integrated over the small energy interval $W_b>W_k\geq 0$; however, a precise analysis of this point is left for future investigation.