

## Generalized Variational Bounds for Multichannel Scatterings

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The variational bounds on scattering parameters are reformulated without the explicit use of multichannel projection operators, thus avoiding completely the difficulty of nonorthogonality in rearrangement and exchange collisions. Resonance-energy calculations can be carried out using the operator which is effectively projected on the closed channels.

### I. INTRODUCTION AND SUMMARY

THE variational bound (VB) on scattering parameters, as originally formulated,<sup>1</sup> employs in an essential way the projection operator technique of Feshbach.<sup>2</sup> Consequently, the difficulty of explicitly deriving such channel projection operators for reaction in which particle exchanges and rearrangements take place severely limits the applicability of VB method.<sup>3</sup> There have been given several alternate derivations<sup>4-8</sup> of VB which eliminate various practical difficulties of carrying out actual calculations and further clarify the basis of the theory.

In this paper, we generalize the previous result by *eliminating* the multichannel projection operators  $P$  and  $Q$  *completely*, so that the method can be applied readily to more complex scattering problems involving exchanges and rearrangements. It is shown that the correct asymptotic boundary conditions alone are *sufficient* to derive the bound. In this connection, the observation of Burke and Taylor<sup>8</sup> in their formulation of VB, that the short-range correlation function need not be orthogonalized to the open channel functions, is most important. The generalization of VB discussed here is equivalent to their point of view, but the present form seems to bring out more clearly, the bound property and the range of applicability. The proof given here is also more direct and explicit.

The generalized VB should then be useful for many interesting scattering systems, such as  $e^+H$  above the pickup threshold,  $e^-He$  and  $e^-$  atom scatterings, and also  $nd$  and  $pd$  scatterings. Thus, so long as the asymptotic conditions (2.2), which involve only  $P_i$  with  $i$

running over all the open channels, can be specified, the result (2.23) is applicable to all possible rearrangement collisions, including the exchanges in case of identical particles. For reactions involving many-particle clusters,  $P_i$  may not be readily available. But this problem is not directly related to the nonorthogonality of the rearrangement channel wave functions, and has to be solved before the scattering problem is considered.

Alternative procedures in which  $G^P$  need not be explicitly evaluated have also been discussed, and certain orthogonality properties of the operators which appear in (2.23) brought out. Finally, a possible way of estimating resonance energies is considered in which the  $Q$  operator is not required.

### II. GENERALIZED VARIATIONAL BOUNDS

For simplicity, we consider explicitly a two-channel problem

$$1 + (2+c) \rightarrow 2 + (1+c), \quad (2.1)$$

where the particles 1 and 2 are distinguishable and  $c$  has no internal structure, but not necessarily an infinite mass. This model contains all the essential properties of more general scattering systems of interest here.

The asymptotic boundary conditions on  $\Psi$  are given by

$$\Psi \rightarrow P_i \Psi_i \quad (2.2)$$

as the channel coordinates  $R_i \rightarrow \infty$ , with  $i=1, 2$ , and where

$$P_i = \psi_0^{(i)}(\mathbf{r}_{jc}) \langle \psi_0^{(i)}(\mathbf{r}_{jc}) \rangle^*,$$

$$P_i^2 = P_i = P_i^\dagger, \quad (2.3)$$

$$Q_i = 1 - P_i, \quad Q_i P_i = 0,$$

$$[P_1, P_2] \neq 0. \quad (2.4)$$

The variational bound as originally formulated<sup>1</sup> assumes an explicit form of the open channel operator  $P$  such that<sup>2</sup>

$$P\Psi = P_1\Psi_1 + P_2\Psi_2 \quad (2.5)$$

and

$$P^2 = P = P^\dagger. \quad (2.6)$$

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<sup>4</sup> R. Sugar and R. Blankenbecler, Phys. Rev. **136**, B472 (1964).

<sup>5</sup> Y. Hahn, Phys. Rev. **139**, B212 (1965), especially Appendix A.

<sup>6</sup> L. Rosenberg, Phys. Rev. **138**, B1343 (1965).

<sup>7</sup> M. Galilitis, Zh. Eksperim. i Teor. Fiz. **47**, 160 (1964)

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<sup>8</sup> P. G. Burke and A. J. Taylor, Proc. Phys. Soc. (London) **88**, 549 (1966).

The knowledge of  $P$  then immediately leads to its complement  $Q$ , given by

$$\begin{aligned} Q &= 1 - P, \\ Q^2 &= Q = Q^\dagger, \quad QP = 0. \end{aligned} \quad (2.7)$$

The physical reason for the bound is essentially that the virtual excitations have an *attractive effect* on scatterings, or, mathematically,

$$Q(H-E)Q > 0 \quad (2.8)$$

for a given total energy  $E$ . Therefore, it seems from (2.8) that the formulation of VB requires the  $Q$  operator in an essential way. However, it is in general extremely difficult to construct such operators explicitly, and  $P_i$  are not simply related to  $P$  due to complicated overlaps.

The variational bound on  $\lambda$  is given by<sup>1</sup>

$$\lambda \leq \lambda_{\mathcal{U}'} = \lambda^P + \Delta_{\mathcal{U}'}, \quad (2.9)$$

where

$$\lambda = 2\pi\hbar^2 \mathbf{a} \cdot K^{-1} \mathbf{a},$$

$$\Delta_{\mathcal{U}'} = 2(Q\Psi_t | QHP | P\Psi^P) + (Q\Psi_t | \mathfrak{C}' - E | Q\Psi_t). \quad (2.10)$$

In (2.9),  $\lambda^P$  is the scattering parameter corresponding to the "static" approximation, and, in (2.10), the vector  $\mathbf{a}$  specifies the initial conditions,  $K^{-1}$  is the inverse reactance matrix, and  $Q\Psi_t$  is a trial function in the  $Q$  space. We also have

$$P(H-E)P\Psi^P = 0, \quad P\Psi^P \equiv \Psi^P, \quad (2.11a)$$

$$P(H-E)PG^P P = -P, \quad PG^P P \equiv G^P, \quad (2.11b)$$

$$\mathfrak{C}' = Q[H + HG^P H]Q = Q\mathfrak{C}'Q. \quad (2.11c)$$

Possible subtraction terms in (2.10) when  $E$  lies above a finite number of eigenstates of  $\mathfrak{C}'$  have been neglected.

Now, we examine (2.10) more closely to see if  $P$  and  $Q$  can be eliminated completely. For this purpose, we first look at the  $P\Psi^P$  Eq. (2.11a) which gives  $\lambda^P$ . Since the explicit form of  $P_i$  is known from the boundary conditions (2.2), we can write, using (2.5),

$$P\Psi^P \equiv P_1\Psi_1^P + P_2\Psi_2^P. \quad (2.12)$$

We also note that  $P$  has the important property (Appendix B)

$$P_i P = P P_i = P_i, \quad (2.13)$$

$$P_i Q = 0, \quad (2.14)$$

although  $P$  is not, in general, a simple linear combination of  $P_i$ . Using (2.13) and (2.14) in (2.11a), we get for  $P\Psi^P$  a coupled set of equations

$$P_1(H-E)P_1\Psi_1^P = -P_1(H-E)P_2\Psi_2^P, \quad (2.15a)$$

$$P_2(H-E)P_2\Psi_2^P = -P_2(H-E)P_1\Psi_1^P. \quad (2.15b)$$

Therefore (2.11a) can be replaced by (2.15), i.e.,

$$P_i(H-E)(P_1\Psi_1^P + P_2\Psi_2^P) = 0 \quad (2.15')$$

for  $i=1, 2$ , where  $P$  does not come in. Similarly, we have, for  $G^P$ ,

$$P_i(H-E)PG^P P = -P_i. \quad (2.16)$$

Solving (2.16) explicitly, we have

$$G^P = G_{11}^P + G_{12}^P + G_{21}^P + G_{22}^P, \quad (2.17)$$

where

$$G_{ij}^P \equiv P_i G_{ij}^P P_j$$

and

$$G_{11}^P = [P_1\{E - H - (H-E)g_2^P(H-E)\}P_1]^{-1},$$

$$G_{12}^P = G_{11}^P(H-E)g_2^P, \text{ etc.}, \quad (2.18)$$

$$g_i^P = [P_i(E-H)P_i]^{-1} = P_i g_i^P P_i. \quad (2.19)$$

(A simple derivation of  $G^P$  is given in Appendix A.) Using the properties (2.7), (2.13), (2.15), and (2.16), we can immediately rewrite (2.10) in the form

$$\begin{aligned} \Delta_{\mathcal{U}'} &= 2(Q\Psi_t | H-E | P\Psi^P) \\ &+ (Q\Psi_t | H-E + (H-E)G^P(H-E) | Q\Psi_t) \\ &= 2(X_t | H-E | P\Psi^P) \\ &+ (X_t | H-E + (H-E)G^P(H-E) | X_t), \end{aligned} \quad (2.20)$$

where  $X_t$  is an arbitrary square-integrable function which satisfies the boundary conditions at the origin, but is *not* necessarily orthogonal to  $P$ . The last equality in (2.20) comes about essentially because  $M$  defined by

$$M \equiv \mathfrak{C}' - E = H - E + (H-E)G^P(H-E) \quad (2.21)$$

is an operator in the  $Q$  space, and

$$N \equiv (H-E)P\Psi^P \quad (2.21')$$

is also a function in the  $Q$  space. That is,

$$\begin{aligned} P_i M &= M P_i = 0, \quad M = Q M Q, \\ P_i N &= 0, \quad N = Q N. \end{aligned} \quad (2.22)$$

Therefore, we finally have the generalized variational bound (GVB) given by

$$\begin{aligned} \lambda &\leq \lambda^P + 2(X_t | H-E | \Psi^P) \\ &+ (X_t | H-E + (H-E)G^P(H-E) | X_t) \\ &\equiv \lambda^P + \Delta_{\mathcal{U}'} = \lambda_{\mathcal{U}'}, \end{aligned} \quad (2.23)$$

where  $\Psi^P$  is given by (2.12), satisfying (2.15);  $G^P$  is given by (2.17), satisfying (2.16); and  $X_t$  is the square-integrable trial function. In the form (2.23), we have eliminated  $P$  and  $Q$  completely, and the only knowledge of the open channels is contained in  $P_i$ . Possible modification due to the presence of a finite number of subtraction terms can be made on (2.23), if necessary.<sup>1</sup>

In order to bring out more closely the effect of nonorthogonal part of  $X_t$  on the bound property of (2.23), we carry out explicitly the proof of the bound using the Kohn variational principle. It has been shown<sup>1</sup> that (2.10) is completely *equivalent* to the Kohn principle

$$[\lambda] = \lambda_t + (\Psi_t | H - E | \Psi_t), \quad \delta[\lambda] = 0 \quad (2.24)$$

if the trial function  $\Psi_t$  in (2.24) is of the specific form

$$\begin{aligned} \Psi_t &= P\Psi^P + G^P P H Q \Psi_t + Q\Psi_t \\ &\equiv P\Psi_t + Q\Psi_t. \end{aligned} \quad (2.25)$$

The error function  $\Omega$  is then given by

$$\begin{aligned} \Omega &\equiv \Psi - \Psi_t \\ &= G^P P H Q \Omega + Q\Omega. \end{aligned} \quad (2.26)$$

Using the Kato identity, we have

$$\begin{aligned} \lambda - \lambda_t &= (\Psi | H - E | \Psi_t) \\ &= (\Psi_t | H - E | \Psi_t) - \tau', \end{aligned} \quad (2.27)$$

where

$$\tau' = (\Omega | H - E | \Omega). \quad (2.28)$$

Substitution of (2.26) into (2.27) and (2.28) gives, after some algebra,

$$\lambda = \lambda^P + \Delta v' - \tau', \quad (2.29)$$

where

$$\tau' = (Q\Omega | \mathcal{H}' - E | Q\Omega), \quad (2.30)$$

and where we have also used

$$\lambda_t = \lambda^P + (Q\Psi_t | QHP | P\Psi^P).$$

Thus, we have

$$\lambda \leq \lambda^P + \Delta v' = \lambda v', \quad (2.31)$$

if

$$\mathcal{H}' - E \geq 0. \quad (2.32)$$

The situation with (2.23) is little more involved; we have, instead of (2.25),

$$\Psi_t = P\Psi^P + F X_t, \quad (2.33)$$

where

$$F = 1 + G^P P (H - E). \quad (2.34)$$

[The form (2.33) is equivalent to requiring that  $P(H - E)\Psi_t = 0$  is solved *exactly* for  $\Psi_t$  in the form  $\psi_t = P\Psi_t + X_t$ . Details are given in Sec. III.] Substitution of (2.33) into (2.24) again gives

$$\lambda = \lambda^P + \Delta v - \tau, \quad (2.35)$$

where  $\Delta v$  is given by (2.20) and

$$\tau = (\Omega | H - E | \Omega) = (\omega | \mathcal{H} - E | \omega) \quad (2.36)$$

with

$$\Omega \equiv \Psi - \Psi_t = F(X - X_t) \equiv F\omega. \quad (2.37)$$

It is clear that  $F$  of (2.34) is an operator which is nonzero only when operated on a  $Q$ -space function,

and thus

$$FP = 0, \quad FQ = F. \quad (2.38)$$

Therefore, if we assume that

$$\mathcal{H} - E = M \geq 0, \quad (2.39)$$

then

$$\tau \geq 0 \quad (2.40)$$

and

$$\lambda \leq \lambda^P + \Delta v = \lambda v. \quad (2.41)$$

We again stress the fact that (2.23) is completely equivalent to (2.24) with (2.33) under the condition (2.39), as was the case with (2.9) being equivalent to (2.24) with (2.25).

The approximate positions of resonances, without the energy-shift operator  $(H - E)G^P(H - E)$ , is often estimated by the Ritz-type variational calculation<sup>9</sup> for the operator  $QHQ$ . Obviously, such a procedure is no longer available since  $Q$  is assumed unknown explicitly. However, from the discussion given above, it is clear that  $M = (\mathcal{H} - E)$  of (2.21) should be a good operator to use for such purpose. For  $E$  below the lowest eigenstate of  $\mathcal{H}$ ,  $M$  is positive definite and thus essentially replaces  $QHQ$  in the resonance energy calculation. The resulting eigenvalues  $M_\mu$  give

$$\varepsilon_\mu^Q = M_\mu + E, \quad (2.42)$$

where the shift effect is taken into account approximately so long as  $G^P(E) \approx G^P(\varepsilon_\mu^Q)$  and  $G^P$  is a slowly varying function of  $E$  near  $E \approx \varepsilon_\mu^Q$ . It is important to keep in mind that  $E$  which appears in the operator  $M$  should all be the *same* in order to stay in the  $Q$  space so that (2.22) is valid. The operator  $M$  should give a better estimate of  $\varepsilon_\mu^Q$  than  $QHQ$  especially when the shifts are large. However,  $G^P$  is in general difficult to construct, although not impossible, and an iterative method of getting  $\varepsilon_\mu^Q$  without an explicit use of  $G^P$  is considered in the next section.

### III. ITERATION PROCEDURE FOR $G^P$

The generalized variational bound (2.23) has been shown to be equivalent to the Kohn variational principle (2.24) with (2.33). However, for practical purposes, both procedures involve  $G^P$  which could be rather involved. In Ref. 5, we have discussed an iterative procedure of avoiding the explicit use of  $G^P$  by replacing (2.25) with an *exact* solution of the differential equations

$$P(H - E)P\Psi_t = -PHQ\Psi_t \quad (3.1)$$

for a given  $Q\Psi_t$ . It is required that  $Q\Psi_t$  is optimized *variationally* by minimizing the expression  $\Delta v$ . For the case of  $e^{-H}$  scattering, Burke and Taylor<sup>8</sup> made an important observation that even (3.1) is unnecessarily strong and in fact an *exact* solution of the equation

$$P(H - E)\Psi_t = 0 \quad (3.2)$$

<sup>9</sup> A. K. Bhatia, A. Temkin, and J. F. Perkins, Phys. Rev. **153**, 177 (1967), where references to earlier work can be found.

is sufficient, without separating  $\Psi_t$  into two parts which requires the explicit form of  $P$  and  $Q$ . Their argument is that one *can* always write (3.1) from (3.2) since  $P+Q=1$ . Of course this is a trivial point if such  $P$  and  $Q$  are explicitly available. However, when they are not, as in most cases of interest, then the advantage of (3.2) over (3.1) in practical calculations is more than a simple identity as it seems. Using (2.13), we can in fact show explicitly below that the exact solution of a set of coupled equations

$$P_i(H-E)\Psi_t=0, \quad i=1, 2 \quad (3.3)$$

combined with the Kohn variational principle (2.24) is completely equivalent to (2.23). To see this, we formally solve (3.3) as

$$\Psi_t = P_1 f_1 + P_2 f_2 + X_t, \quad (3.4)$$

where

$$P_i f_i = P_i \Psi_t^P + (G_{ii}^P + G_{ij}^P)(H-E)X_t, \quad i \neq j \quad (3.5)$$

and  $X_t$  is again a square-integrable function but *not* necessarily orthogonal to both  $P_1$  and  $P_2$ . Thus,  $\Psi_t$  of (3.4) is exactly the form (2.33), and the proof of the bound is then identical to the one given in Sec. II; we obtain the same result (2.23) as expected. In so far as the practical procedure is concerned, (3.3) combined with (2.24) may be much simpler than (2.23) since we do not have to solve for  $G^P$  explicitly. We let

$$X_t = \sum_{i=1}^N c_i X_{it}(\alpha), \quad (3.6)$$

where  $c_i$  are the linear parameters and  $\alpha$  is one of the nonlinear parameters. For a fixed value of  $\alpha$ ,  $c_i$  can be determined from the equation

$$\sum_j (H_{ij} - EN_{ij})c_j = -R_{1i} - R_{2i}, \quad (3.7)$$

where

$$H_{ij} = (X_{it}, HX_{jt}), \quad N_{ij} = (X_{it}, X_{jt}), \\ R_{1i} = (X_{it}, [H-E]P_1 f_1).$$

By simultaneously diagonalizing the energy matrix and the normalization matrix, we get

$$X_t = \sum_{\mu=1}^N \frac{|X_{\mu t}\rangle \langle X_{\mu t}^*|}{E - E_{\mu t}(\alpha)} [H-E](P_1 f_1 + P_2 f_2). \quad (3.8)$$

Substitution of (3.8) into (3.3) gives the coupled equations for  $P_1 f_1$  and  $P_2 f_2$  which are to be solved *exactly*. We have explicitly included the  $\alpha$  dependence of  $E_{\mu t}$  in (3.8). Thus, we have

$$P_i(H-E)P_i f_i + \sum_{\mu=1}^N \frac{P_i(H-E)|X_{\mu t}\rangle \langle X_{\mu t}|(H-E)}{E - E_{\mu t}(\alpha)} P_i f_i \\ = -P_i \left[ H-E + \sum_{\mu=1}^N (H-E) \frac{|X_{\mu t}\rangle \langle X_{\mu t}|}{E - E_{\mu t}(\alpha)} (H-E) \right] P_i f_i, \quad (3.9)$$

where  $i \neq j$ . For each value of  $\alpha$ , the diagonalization of  $H_{ij}$  has to be repeated, and (3.9) solved *exactly*. The resulting parameters then are a bound as in (2.23), essentially due to (2.38). This iteration procedure should converge for most cases.<sup>5</sup> It requires some caution, however, in applying (3.9) in an extensive search for the "best"  $\alpha$  which gives the minimum  $\lambda_V$ . Since  $X_{it}$  are *not* preorthogonalized to the  $P$  space,  $E - E_{\mu t}(\alpha)$  may vanish occasionally as  $\alpha$  is swept over a range of values. So long as such spurious singular points are avoided, the procedure outlined above is the same as (2.23). In this connection, we mention a procedure proposed recently by Harris,<sup>10</sup> precisely to overcome such singularities. The main point is to choose

$$E = E_{\mu t}, \quad \mu = 1, \dots, N \quad (3.10)$$

and writing

$$X_t = \sum_{\mu=1}^N a_{\mu} X_{\mu t}, \quad (3.11)$$

we obtain, for the original equation  $(H-E)\Psi_t=0$ ,

$$\langle X_{\mu t} | H-E | P_1 f_1 \rangle + \langle X_{\mu t} | H-E | P_2 f_2 \rangle = 0. \quad (3.12)$$

Equation (3.12) is sufficient to estimate the scattering parameters. Of course, the bound property is *lost* since  $P_1 f_1$  and  $P_2 f_2$  are *not obtained exactly*, i.e., the  $P$  equations are not solved exactly for  $P_i f_i$ .

Finally, we consider a possible way of eliminating  $G^P$  in the resonance energy calculation. If we define  $P y_{it}$ , for each  $X_{it}$ , by the equations

$$P(H-E)P y_{it} = -P(H-E)X_{it} \quad (3.13)$$

exactly such that

$$P y_{it} \rightarrow (\text{const})_i G^P, \quad (3.14)$$

then the matrix elements needed to evaluate the resonance energies are given by

$$M_{ij} = (X_{it} | M | X_{jt}) \\ = (X_{it} | H-E | X_{jt}) + (X_{it} | H-E | P y_{jt}). \quad (3.15)$$

It is now a simple matter to diagonalize  $M_{ij}$ , with the added feature that  $M_{ij}$  never vanishes (all the eigenvalues are positive definite). This is perhaps an improvement over the procedure of Ref. 8.

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<sup>10</sup> F. E. Harris, Phys. Rev. Letters **19**, 173 (1967).

### APPENDIX A: STATIC GREEN'S FUNCTION $P^P$

The static Green's function  $G^P$  which satisfies (2.11b) assumes the form (2.7) if there exists<sup>2</sup> an operator  $P$  which satisfies (2.12)–(2.14). Equation (2.16) can be written as

$$P_1(H-E)(G_{11}^P+G_{21}^P) + P_1(H-E)(G_{12}^P+G_{22}^P) = -P_1, \quad (\text{A1})$$

$$P_2(H-E)(G_{22}^P+G_{12}^P) + P_2(H-E)(G_{21}^P+G_{11}^P) = -P_2, \quad (\text{A2})$$

where  $G_{ij}^P$  are yet undefined. Since, for example,  $G_{12}^P$  and  $G_{22}^P$  in (A1) involve  $P_2$  on their right, we rewrite (A1) and (A2) in the form

$$P_1(H-E)G_{11}+P_1(H-E)G_{21} = -P_1, \quad (\text{A3})$$

$$P_1(H-E)G_{12}+P_1(H-E)G_{22} = 0, \quad (\text{A4})$$

and

$$P_2(H-E)G_{22}+P_2(H-E)G_{12} = -P_2, \quad (\text{A5})$$

$$P_2(H-E)G_{21}+P_2(H-E)G_{11} = 0. \quad (\text{A6})$$

The above separation is justified since, from (2.13), the  $P_2$  part of  $P$  can always be incorporated in (A5) and not in (A4), and similarly for  $P_1$ . Now (A3) is coupled to (A6) and (A5) is coupled to (A4). The solution is trivially obtained to be the form (2.18). The step leading to (A3)–(A6) from (A1) and (A2) can be shown to be correct in another way by solving a coupled inhomogeneous equation

$$P(H-E)Pf = -PR. \quad (\text{A7})$$

Using the fact that

$$Pf \equiv P_1f_1 + P_2f_2, \\ PR = P_1R_1 + P_2R_2, \quad (\text{A8})$$

we have

$$P_1\bar{\Psi}f_1 = P_1\Psi^P + G_{11}^P(H-E)P_2\Psi^{P2} + (G_{11}^P + G_{12}^P)PR, \quad (\text{A9})$$

where

$$[G_{11}^P]^{-1}P_1\bar{\Psi}^P = 0, \quad [g_1^P]P_1\Psi^{P1} = 0.$$

On the other hand, we formally have

$$Pf = P\Psi^P + G^P PR \quad (\text{A10})$$

with

$$P_1\Psi_1^P = P_1\bar{\Psi}^P + G_{11}^P(H-E)P_2\Psi^{P2}, \\ P\Psi^P \equiv P_1\Psi_1^P + P_2\Psi_2^P.$$

Comparing (A9) with (A10), we recover (2.17).

### APPENDIX B: PROJECTION OPERATORS $P_i$ AND $P$

The crucial properties of the projection operators which were used in the derivation of the generalized

variational bound (2.23) are (2.13) and (2.14), and we give here a brief discussion of their validity.

From one of the requirements that  $P$  must satisfy in constructing it from  $P_i$  [Eq. (2.5)], we have, in the case of two channels, for example,

$$(P_i, [\Psi - (P_1\Psi_1 + P_2\Psi_2)]) = 0, \quad (\text{B1})$$

or

$$(P_i, Q\Psi) = 0, \quad (\text{B2})$$

which is simply (2.14). Now, (2.14) in turn gives

$$P_i Q = P_i(1-P) = 0, \quad (\text{B3})$$

or simply

$$P_i P = P_i, \quad (\text{B4})$$

as it should. Using the Hermiticity property (2.3), we also have

$$P P_i = P_i. \quad (\text{B5})$$

There are several cases for which  $P$  and  $P_i$  are explicitly available. First, we have the  $e^-H$  elastic scattering in which<sup>1</sup>

$$P = P_1 + P_2 - P_1 P_2 = P_1 + P_2 - P_2 P_1, \\ Q = 1 - P = Q_1 Q_2 = Q_2 Q_1. \quad (\text{B6})$$

Obviously, both (B4) and (B5) are satisfied.

Second, we have the explicit  $P$  for the  $e^+H$  elastic and pickup collisions given by Mittleman,<sup>11</sup> as derived by the procedure worked out by Feshbach,<sup>2</sup>

$$P = \psi_0 \left[ \delta(\mathbf{r} - \mathbf{r}') + \sum_{\lambda} \frac{u_{\lambda}}{\lambda^2 - 1} \langle u_{\lambda}^* \rangle \right] \langle \psi_0^* + \sum_{\lambda} \psi_0 u_{\lambda} \rangle \frac{\lambda}{\lambda^2 - 1} \\ \times \langle v_{\lambda}^* \phi_0^* + \sum_{\lambda} \phi_0 v_{\lambda} \rangle \frac{\lambda}{\lambda^2 - 1} \langle u_{\lambda}^* \psi_0^* + \phi_0 \rangle \\ \times \left[ \delta(\mathbf{p} - \mathbf{p}') + \sum_{\lambda} \frac{v_{\lambda}}{\lambda^2 - 1} \langle v_{\lambda}^* \rangle \right] \langle \phi_0^* \rangle, \quad (\text{B7})$$

where  $\psi_0(\mathbf{r})$  is the hydrogenic ground-state wave function and  $\phi_0(\mathbf{p})$  is for the positronium.  $u_{\lambda}$  and  $v_{\lambda}$  are solutions of the coupled equations

$$u_{\lambda} + \lambda K_1 v_{\lambda} = 0, \\ v_{\lambda} + \lambda K_2 u_{\lambda} = 0, \quad (\text{B8})$$

with

$$K_1 = 8\psi_0^*, \quad \phi_0 = K_2^+ = - \sum_{\lambda} \lambda^{-1} u_{\lambda} v_{\lambda}^*. \quad (\text{B9})$$

Defining the channel operators  $P_i$ ,  $i=1, 2$ , as

$$P_1 = \psi_0 \langle \psi_0^* \rangle, \quad P_2 = \phi_0 \langle \phi_0^* \rangle, \quad (\text{B10})$$

we can show, after some algebra using (B8)–(B10), that (B4) and (B5) are again satisfied.

<sup>11</sup> M. H. Mittleman, Ann. Phys. (N.Y.) **28**, 430 (1964).