Formulation of elastic and inelastic breakup-fusion reactions

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The calculations, presented earlier for the elastic breakup-fusion reactions, is extended here to include inelastic breakup-fusion reactions. As we did before, we take the necessary precautions to eliminate unphysical contributions, which are otherwise mixed into the breakup amplitudes, due to the nonorthogonality between wave functions in the entrance and breakup channels. Related theories by Ichimura *et al.*, and by Hussein and McVoy, are also discussed and it is shown that they retain such unphysical contributions.

I. INTRODUCTION

As is well known, the multistep direct reaction (MSDR) theory has been successful in analyzing a variety of data for reactions induced by both light and heavy ions. Earlier, the theory was applied exclusively to reactions that lead to discrete final states.¹ More recently, the theory has been extended to analyze continuum reaction data.²⁻⁴

As is expected, however, the MSDR alone cannot explain all the observed data. In fact, there have been observed reactions in which the direct and compound mechanisms do seem to play interwoven roles. These are reactions that have been called by several different names: incomplete fusion,⁵ massive transfer,⁶ or breakup-fusion $(BF)^7$ reactions.

Take as an example the (α, p) reaction.^{8,9} The forward peaked angular distribution of the continuum protons indicates that they were produced via a direct reaction. However, the coincidence measurement of these protons with γ rays demonstrates that the rest of the system, i.e., the triton plus the target, form a compound system. Similar features have been seen in many other reactions.^{5,6,10}

In our recent publications, 1^{1-15} we have described these reactions as BF reactions. Such reactions proceed in two stages, the first stage being a direct breakup reaction, and the second stage a (partial) fusion. The reaction may thus be viewed as an incomplete fusion. (Reference 11 by Udagawa and Tamura, in which the initial formalism of our BF calculation was presented, will henceforth be referred to as UT.)

The formulation to calculate the BF reaction cross sections was given in Ref. 11, restricted, however, to the simplest type of BF, i.e., EBF, in which the first stage breakup is a pure one-step elastic breakup (EB). The EB means that all the particles produced in the reaction (i.e., the target and the broken up pairs) remain in their ground states. Because of this simplification, we were able to derive a very simple cross section formula,¹¹ which turned out to be identical to that derived earlier by Kerman and McVoy in a quite different way.¹⁶

Using the formula, we have carried out extensive numerical calculations for light ion induced reactions, i.e., the (α, p) , (α, d) , (α, t) , (h, p), and (h, d) reactions.^{13,14} In spite of the fact that only the EBF contributions were in-

cluded, the calculations were able to explain rather well the experimental spectra, at least at higher energies. It is remarkable that these calculations well reproduce the absolute magnitude of the experimental cross sections.¹¹⁻¹⁴

We nevertheless found that the simple EBF calculation underestimated systematically the lower energy part of the (singles) spectra. The discrepancies are particularly large for massive transfer-type reactions such as (α, p) and (h,p). We have ascribed these discrepancies to higher order processes neglected in the EB and EBF calculations.

The major purpose of the present paper is to extend our previous BF theory¹¹ so as to include higher order effects, particularly inelastic scattering effects. More specifically, we consider the target excitations taking place simultaneously with or in advance of the breakup. We may call these reactions the inelastic BF (IBF) reactions. We shall derive cross section formulas, similar to those derived¹¹ for the EBF reaction.

In deriving the IBF (as well as EBF) cross section formulas, it is important to keep in mind that great caution has to be exercised so as not to include *unphysical contributions*. The amplitude for the inelastic breakup (IB) reaction often includes the amplitude for the *pure inelastic scattering*, which is unphysical and thus has to be eliminated. It seems to us that this problem is not so well known, and we intend to discuss it in detail in this paper.

After presenting our IB and IBF formulas in Sec. II, we discuss in Sec. III the BF theory of Ichimura, Austern, and Vincent (IAV).¹⁷ They claim that their BF formula includes inelastic, as well as elastic, breakup effects. As seen in Sec. III, we agree with IAV in this regard. However, we show at the same time that their IBF cross section includes *unphysical* (inelastic scattering) contributions, which should have been eliminated. A cross section formula very similar to that of IAV was also obtained by Hussein and McVoy (HM),¹⁸ and we shall also discuss it in Sec. III.

II. FORMULATION OF THE CALCULATIONS

A. Introductory remarks

The EBF reaction considered in our previous studies $^{11-15}$ may symbolically be written as

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$$a + A \rightarrow b + x + A \rightarrow b + B^* . \tag{2.1}$$

In (2.1) in which each step is indicated by an arrow, the first step is an EB of the projectile a into b + x, while the second step is the fusion of x into the target A to form a compound nucleus B^* ; b is simply emitted. Throughout the present paper, we are interested in calculating singles cross section for observing b. Henceforth, we shall call the systems, consisting of x and A, and b and B^* , respectively, the x and b channels. The incident channel consisting of a and A will be called the a channel.

It is clear that the above EBF is the simplest among many conceivable BF reactions. As emphasized in the Introduction, we consider, in the present paper, also IBF reactions, in which the fusion step is preceded by inelastic breakup (IB) steps. More concretely, we consider the following two processes;

$$a + A \rightarrow b + x + A^* \rightarrow b + B^*$$
, (2.2a)

$$a + A \rightarrow a' + A^* \rightarrow b + x + A^* \rightarrow b + B^*$$
. (2.2b)

As seen, they involve the excitation of A into A^* .

In the process in (2.2a), the first step is still a one-step breakup reaction, but contrary to that in (2.1) it involves a simultaneous excitation of the target and the projectile. We may call this a simultaneous-IB (Sim-IB) process. The whole process of (2.2a), which we may call Sim-IBF, has an appearance of being a two-step process.

In the process in (2.2b), inelastic scattering takes place first and breakup follows. We may call this two-step process a successive-IB (Suc-IB). The whole process of (2.2b) may then be called Suc-IBF; it has the form of a threestep process.

In the hierarchy of the Born expansion, the Sim-IB is in fact a second Born, rather than a first Born process. One will see this clearly, if one notes that EB can be regarded as an inelastic excitation of a into its continuum (states). In the discrete state transition problems,¹⁹ it is customary to treat both the simultaneous and successive excitations of the projectile and the target as second Born processes. We follow this practice here, and consider the two processes in (2.2a) and (2.2b) to be of the same order.

It is important to keep in mind that the states reached in (2.2a) and (2.2b), before the final fusion takes place, may be the same. If this occurs, the amplitudes of the two processes must be added coherently.

An important aspect we employ in our formulation of the present study is that we treat b as a spectator, i.e., we make a spectator approximation.¹¹ More explicitly, we describe the motion of b relative to B^* in terms of an optical model wave function, $\chi_b^{(-)}$. Thus b does not participate explicitly in what happens in B^* , except that it is elastically scattered and also absorbed by B^* in the usual sense of the optical model.

B. Notations and basic relations

As seen from (2.1) and (2.2), we encounter nuclei a, A, b, x, and B, which we collectively denote by i. The inter-

nal (intrinsic) Hamiltonian, internal wave function, and the eigenenergy of the nucleus *i* will be denoted by h_i , ϕ_i , and e_i , respectively. We thus have a relation that

$$h_i \phi_i = e_i \phi_i \quad (i = a, A, b, x, \text{ and } B)$$
(2.3)

The eigenfunction and eigenenergy of excited states of *i* will be denoted by ϕ_{i*} and e_{i*} .

As we have explained, in relation to (2.1) and (2.2), we encounter a few two-body channels, i.e., the *a*, *x*, and *b* channels, which we shall denote collectively by *j*. The kinetic energy operator, the optical model potential, and the energy for the channel *j* will be denoted by T_j , U_j , and E_j , respectively. By defining further $K_j = T_j + U_j$, we thus have a relation that

$$(E_j - K_j)\chi_j^{(\pm)} = 0 \ (j = a, b, \text{ and } x)$$
. (2.4)

The distorted wave $\chi_j^{(+)}$ is used for j = a, while $\chi_j^{(-)}$ is used for j = b and x.

The total energy of the whole system will be denoted by E. We then have the relations that

$$E_a = E - (e_a + e_A) , \qquad (2.5)$$

$$E_{x} = E_{a} - E_{b} + (e_{a} + e_{A} - e_{b} - e_{x} - e_{A^{*}}) . \qquad (2.6)$$

Clearly, E_a is the incident energy, while E_x is the kinetic energy of x, the quantity in the parentheses in (2.6) being the Q value for the breakup process. If EB takes place, we of course have $e_{A*}=e_A$.

After defining various quantities in this way, we now present a few basic relations, obtained within the projection operator formalism of Feshbach.^{20,21} We assume that the P space includes all the elastic and open inelastic channels. The projection operator P may then be given as

$$P = p_a P_A \quad (Q = 1 - P) , \qquad (2.7)$$

with

$$p_a = |\phi_a\rangle\langle\phi_a| \quad , \tag{2.8a}$$

$$P_{A} = \sum_{A^{*}} \langle \phi_{A^{*}} \rangle \langle \phi_{A^{*}} | .$$
(2.8b)

The symbol \sum' indicates that the sum of A^* should be taken only over the open excited channels. The total reaction cross section σ_R may then be given as a sum of the total inelastic scattering cross section σ_{IN} , and the rest, which we shall denote by σ'_R . Note that the breakup and BF cross sections are of course contained in σ'_R . In what follows, we shall thus concentrate our interest only on σ'_R . What will actually be done is to extract the breakup and BF cross sections from σ'_R .

Explicitly, σ'_R can be given as^{20,21}

$$\sigma_{R}^{\prime} = (2\pi/\hbar v_{a}) \left[-\operatorname{Im} \left\langle \Psi_{P} \left| H_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} H_{QP} \left| \Psi_{P} \right\rangle \right/ \pi \right]$$

where v_a is the velocity of *a* relative to *A*, while the meaning of $H_{QQ} = QHQ$, H_{QP} $(=V_{QP}) = QHP$, etc., is well known.^{20,21} Also, Ψ_P is the *P*-channel part of the total wave function of the system, $\Psi_a^{(+)}$, i.e., $\Psi_P = P\Psi_a^{(+)}$. Ψ_P satisfies

$$(E - H_P)\Psi_P = 0$$
, (2.10)

where

$$H_{P} = h_{a} + h_{A} + T_{a} + U_{P}$$

= $h_{b} + h_{x} + h_{A} + T_{xb} + V_{xb} + T_{a} + U_{P}$, (2.11)

with

$$U_{P} = V_{PP} + V_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} V_{QP} . \qquad (2.12)$$

V in (2.12) is the interaction potential in the channel a; i.e., the prior form of the interaction.

As is well known, it is customary to interpret the energy average of Ψ_P as a direct reaction model wave function. We thus take it here as a coupled-channel (CC) model wave function. Likewise, we take the energy average of U_P as the CC potential. With these interpretations, Ψ_P can now be given as a sum of the elastic and inelastic channel wave functions as

$$\Psi_{P} = \sum_{A^{*}} \Phi_{a'A^{*}}^{(+)} \quad \text{with} \quad \Phi_{a'A^{*}}^{(+)} = \chi_{a'A^{*}}^{(+)} | \phi_{a} \phi_{A^{*}} \rangle .$$
 (2.13)

If (2.13) is inserted into (2.10), the latter becomes a CC equation for determining $\chi_{a'A^{\ddagger}}^{(+)}$, and there is no intrinsic difficulty in solving this equation. For the purpose of the present paper to calculate *b*-singles cross section, however, it makes more sense to avoid solving this CC equation as it stands, and to resort to a perturbative approach in evaluating $\chi_{a'A^{\ddagger}}^{(+)}$. Then, the elastic component $\chi_{aA}^{(+)}$ is approximated by the distorted wave function $\chi_{a}^{(+)}$, cf. Eq. (2.4), while the excited channel wave function as

$$\Phi_{a'A}^{(+)} = G_a(\phi_a \phi_A * | U'_a | \Phi_{aA}^{(+)}\rangle \quad (\Phi_{aA}^{(+)} = \chi_a^{(+)} \phi_a \phi_A) .$$
(2.14)

In (2.14), the integration symbol $(| | \rangle)$ was used to indicate that the integration is performed by keeping the *a*-channel coordinate \mathbf{r}_a fixed. Also, G_a is the Green's function in the *a* channel and is defined as

$$G_a = \frac{1}{E_a - H_a + i\epsilon} , \qquad (2.15a)$$

with

$$H_a = h_a + h_A + T_a + U_a \ . \tag{2.15b}$$

The U'_a and U_a involved in (2.14) and (2.15) are the diagonal and nondiagonal parts of U_P ;

$$U_P = U_a + U'_a \quad , \tag{2.15c}$$

and U_a in particular is identified as the optical model potential that appeared in (2.4).

We shall now take an important step by noting that the operator part of (2.9) can be rewritten, as proved in Appendix A, as

$$V_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} V_{QP} = P V_P^{\dagger} G V_P P , \qquad (2.16)$$

where

$$G = \frac{1}{E - H + i\epsilon} , \qquad (2.17)$$

and

$$V_P = V - U_P$$
 . (2.18)

Using (2.16), (2.9) can now be rewritten as

$$\sigma_{R}^{\prime} = (2\pi/\hbar v_{a})(-\operatorname{Im}\langle\Psi_{P} \mid V_{P}^{\dagger} G V_{P} \mid \Psi_{P} \rangle/\pi) . \quad (2.19)$$

As already remarked, σ'_R does not contain any part of the elastic and inelastic cross sections. This is evident from our original definition of σ'_R [cf. (2.9)], in which the Q operator took care of eliminating these cross sections. It is then important to note that the role which Q played in (2.9) is now played by U_P , which has been subtracted from V to form V_P [cf. (2.18)]. To see this, let us represent the (exact) Green's function in (2.19) by a complete set of the exact wave functions, $\Psi'_B^{(-)}$, as

$$G = \sum_{\beta} |\Psi_{\beta}^{(-)}\rangle \frac{1}{E - E_{\beta} + i\epsilon} \langle \Psi_{\beta}^{(-)}| \quad .$$
 (2.20)

The possible contributions to the elastic and inelastic scattering come from the terms, in which $\beta = (a'A^*)$. However, these possible contributions are in fact nil. In fact, for $\beta \in P$, we have [with the help of $Q\Psi_{\beta}^{(-)} = (E - H_{QQ} - i\epsilon)^{-1}V_{QP}\Psi_{\beta}^{(-)}$]

$$\langle \Psi_{\beta}^{(-)} | V_{P} | \Psi_{P} \rangle = \langle \Psi_{\beta}^{(-)} | V - U_{P} | \Psi_{P} \rangle = \left\langle P \Psi_{\beta}^{(-)} \right| V_{PP} + V_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} V_{QP} - U_{P} \left| \Psi_{P} \right\rangle = 0.$$
(2.21)

(2.9)

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Later, towards the end of Sec. IIE, we shall discuss the importance of relation (2.21).

C. Approximations

Equation (2.19) is exact, and is much handier than is (2.9), but cannot yet be used as it stands for actual calculations. In order to make use of (2.19) for practical purpose, we shall now introduce a few approximations. The first step of the approximations to make is to replace the exact Green's function G in (2.19) by G_d ; we set

$$G \simeq G_d$$
 . (2.22)

This G_d is the Green's function in the breakup channel d, and is given by

$$G_d = \frac{1}{E - (h_b + h_x + h_A + K_b + K_x) + i\epsilon}$$
 (2.23)

By using (2.22), σ'_R is now reduced to

$$\sigma_R' = (2\pi/\hbar v_a)(-\operatorname{Im}\langle \Psi_P \mid V_P^{\dagger} G_d V_P \mid \Psi_P \rangle / \pi) . \qquad (2.24)$$

This relation is essentially the same as that used in Ref. 11; see Eq. (3) of Ref. 11. The only difference is that the CC wave function Ψ_P and the CC potential U_P are involved in (2.24), while the elastic channel wave function and the optical model potential are as they appear in Eq. (3) of Ref. 11. The rest of the formulation can thus be done in very much the same way as in Ref. 11.

We now note that it is easy to prove the identity that

$$G_{d} = \Omega_{b}^{(-)} [E - (T_{b} + h_{b} + h_{x} + h_{A} + K_{x}) + i\epsilon]^{-1} \Omega_{b}^{(-)^{\dagger}} - G_{d}^{\dagger} U_{b}^{\dagger} G_{d} , \qquad (2.25a)$$

where the wave operator $\Omega_b^{(-)}$ is given as

$$\Omega_b^{(-)} = 1 + G_d^{\dagger} U_b^{\dagger} . \qquad (2.25b)$$

By using (2.25a), it is clear that σ'_R can now be divided

into two terms as

$$\sigma_R' = \sigma_R^{(1)} + \sigma_R^{(2)} , \qquad (2.26)$$

with

$$\sigma_R^{(1)} = (2\pi/\hbar v_a) (-\operatorname{Im} \langle \Psi_P | V_P^{\dagger} G_{\mathbf{x}, b} V_P | \Psi_P \rangle / \pi) , \quad (2.27a)$$

$$\sigma_R^{(2)} = (2\pi/\hbar v_a) (\langle G_d V_P \Psi_P | W_b | G_d V_P \Psi_P \rangle / \pi) , \quad (2.27b)$$

where

$$G_{x,b} = \Omega_b^{(-)} [E - (T_b - h_b - h_x + h_A + K_x) + i\epsilon]^{-1} \Omega_b^{(-)^{\dagger}}.$$
(2.28)

As seen, $\sigma_R^{(2)}$ in (2.27b) is in the form of an expectation value of W_b (with respect to the wave function $|G_d V_P \Psi_P\rangle$), and hence is a cross section for absorbing b. In other words, $\sigma_R^{(2)}$ does not contribute to the cross section for observing b.

The cross section for observing b is contained in $\sigma_R^{(1)}$ and, in order to bring it into a tractable form, we now make the second of the approximations; i.e., the spectator approximation. As was explained at the end of Sec. II A, this approximation is to assume that the state of b can be well described by the distorted wave function $\chi_b^{(-)}$. To make this spectator approximation is equivalent to approximating $\Omega_b^{(-)}$ in Eq. (2.28) by the optical model wave operator $\omega_b^{(-)}$ which is given as

$$\omega_{b}^{(-)} \equiv 1 + (E_{b} - T_{b} - U_{b}^{\dagger} - i\epsilon)^{-1} U_{b}^{\dagger} . \qquad (2.29)$$

Note that $\Omega_b^{(-)}$ of (2.26) contains G_d , which is a threebody channel propagator [as seen from its definition given in (2.23)]. On the other hand, $\omega_b^{(-)}$ of (2.30) contains a two-body channel propagator $(E_b - T_b - U_b^{+} - i\epsilon)^{-1}$. Because of this replacement, the calculation has now become tractable, and the nature of the approximation we have made will thus be very clear.

The $G_{x,b}$ of (2.28) is now rewritten as

$$G_{x,b} = \sum_{\mathbf{k}_{b}x^{*}b^{*}A^{*}} \omega_{b}^{(-)} | \phi_{b,x} \rangle \langle \phi_{b,x} | (E - T_{b} - h_{b} - h_{x} - h_{A} - K_{x} + i\epsilon)^{-1} | \phi_{b,x} \rangle \langle \phi_{b,x} | \omega_{b}^{(-)^{\dagger}} , \qquad (2.30a)$$

where we have inserted the complete set of wave functions $\phi_{b,x}$, which are defined by

$$|\phi_{b,x}\rangle = \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{k}_b \cdot \mathbf{r}_b) |\phi_{b*}\phi_{x*}\phi_{A*}\rangle . \quad (2.30b)$$

The factor $\exp(i\mathbf{k}_b \cdot \mathbf{r}_b)$ in (2.30b) is a plane wave in the *b* channel. Since

$$\omega_{\boldsymbol{b}}^{(-)} \exp(i\mathbf{k}_{\boldsymbol{b}} \cdot \mathbf{r}_{\boldsymbol{b}}) = \chi_{\boldsymbol{b}}^{(-)}, \qquad (2.31a)$$

and

$$(E - T_b - h_b - h_x - h_A - K_x + i\epsilon)^{-1} |\phi_{b,x}\rangle$$

= $(E_x - K_x + i\epsilon)^{-1} |\phi_{b,x}\rangle$, (2.31b)

we see that (2.30a) is now rewritten as

$$G_{x,b} = \sum_{k_b x^{*}_b *_A *} \frac{1}{(2\pi)^3} | \phi_{x^*} \phi_{b^*} \phi_{A^*} \chi_b^{(-)} \rangle \times G_x(\chi_b^{(-)} \phi_{x^*} \phi_{b^*} \phi_{A^*} | , \qquad (2.32a)$$

where the symbols $| \rangle$ and (| were used to indicate that the state vectors are not for the complete a + A system, but exclude the radial component of the x-channel wave function. Also,

$$G_{\mathbf{x}} = \frac{1}{E_{\mathbf{x}} - K_{\mathbf{x}} + i\epsilon} \quad (2.32b)$$

In (2.32), E_x is the kinetic energy of x as was defined in (2.6). Note that G_x of (2.32a) is again a two-body propa-

gator, and thus is tractable. Note also that the sum over b^* , x^* , and A^* in (2.32a) are extended over all the excited states of b, x, and A, including their ground states.

D. BF cross section formulas

Since, in the present paper, we discuss the breakup reactions induced by light ions, we shall suppress the sum over b^* and x^* in the expression of (2.32a); both b and x can be considered to remain in their respective ground states.

Let us now rewrite $\sigma_R^{(1)}$ of (2.27a) further. To do this, we use (2.32a) (after suppressing the sum over b^* and x^*), and also an identity given by

$$-\operatorname{Im} G_{\mathbf{x}} = -\omega_{\mathbf{x}}^{(-)} \left[\operatorname{Im} \frac{1}{E_{\mathbf{x}} - T_{\mathbf{x}} + i\epsilon} \right] \omega_{\mathbf{x}}^{(-)^{\dagger}} + G_{\mathbf{x}}^{\dagger} W_{\mathbf{x}} G_{\mathbf{x}} .$$
(2.33)

Here $\omega_x^{(-)}$ is the wave operator for the x channel. [The derivation of (2.33) is the same as that of (2.25a).]

We now have

$$\sigma_{R}^{(1)} = \int dE_{b} d\Omega_{b} \left[\int d\Omega_{x} \frac{d^{3} \sigma^{B}}{dE_{b} d\Omega_{b} d\Omega_{x}} + \frac{d^{2} \sigma^{BF}}{dE_{b} d\Omega_{b}} \right],$$
(2.34)

where

$$\frac{d^{3}\sigma^{B}}{dE_{b}d\Omega_{b}d\Omega_{x}}$$

$$=(2\pi/\hbar v_{a})\rho(E_{b})\rho(E_{x})\frac{1}{2s_{a}+1}$$

$$\times \sum_{A^{*}m_{b}m_{x}m_{a}}|\langle \chi_{x}^{(-)}\chi_{b}^{(-)}\phi_{x}\phi_{b}\phi_{A^{*}}|V_{P}|\Psi_{P}\rangle|^{2},$$
(2.35a)

$$\frac{d^{2}\sigma^{\rm BF}}{dE_{b}d\Omega_{b}} = (2\pi/\hbar v_{a})\rho(E_{b})\frac{1}{(2s_{a}+1)} \times \sum_{A^{*}m_{b}m_{x}m_{a}} (\langle \psi_{xA^{*}}^{(+)} | W_{x} | \psi_{xA^{*}}^{(+)} \rangle/\pi) . \quad (2.35b)$$

The x-channel wave function $\psi_{xA^*}^{(+)}$ is defined as

$$\psi_{xA^{*}}^{(+)} = G_{x}(\chi_{b}^{(-)}\phi_{b}\phi_{x}\phi_{A^{*}} | V_{P} | \Psi_{P} \rangle .$$
(2.36)

The factor $\rho(E_b)$ that appears in the above equations is the phase space volume of the emitted particle *b*, and $\rho(E_x)$ is the same quantity for *x*.

The cross section given by (2.35a) is that for breakup, i.e., the processes in which both x and b are emitted. On the other hand, that in (2.35b) is for BF, in which only b is emitted, and x is absorbed.

The EBF cross section can now be obtained by picking the ground state A for A^* in (2.35b). It is thus written as

$$\frac{d^2 \sigma^{\text{EBF}}}{dE_b d\Omega_b} = (2\pi/\hbar v_a) \rho(E_b) \frac{1}{2s_a + 1}$$

$$\times \sum_{m_b m_x m_a} (\langle \psi_x^{(+)} | W_x | \psi_x^{(+)} \rangle / \pi) , \quad (2.37)$$

where

$$\psi_{\mathbf{x}}^{(+)} \equiv \psi_{\mathbf{x}A}^{(+)} = G_{\mathbf{x}}(\chi_{b}^{(-)}\phi_{b}\phi_{\mathbf{x}}\phi_{A} \mid V_{P} \mid \Psi_{P})$$
$$\simeq G_{\mathbf{x}}(\chi_{b}^{(-)}\phi_{b}\phi_{\mathbf{x}}\phi_{A} \mid V_{a} \mid \Phi_{aA}^{(+)}), \qquad (2.38a)$$

with

$$V_a = V - U_a \quad . \tag{2.38b}$$

In obtaining the last (near) equality in (2.38a), we replaced Ψ_P by $\Phi_{aA}^{(+)}$, i.e., we neglected the inelastic component in Ψ_P . (It gives a higher order contribution.) Once this is done, we can replace V_P by V_a , because the coupling term U'_a in V_P does not contribute to the matrix element in the last line of (2.38a). The EBF cross section obtained as (2.37) is exactly the same as what was given earlier in Ref. 11. It was used in the studies in Refs. 12–15.

The terms in (2.35b) in which $A^* \neq A$ give the IBF cross sections. Explicitly, it is given as

$$\frac{d^2 \sigma^{\text{IBF}}}{dE_b d\Omega_b} = (2\pi/\hbar v_a) \rho(E_b) \frac{1}{2s_a + 1}$$

$$\times \sum_{A^*M_A * m_b m_x m_a} (\langle \psi_{xA^*}^{(+)} | W_x | \psi_{xA^*}^{(+)} \rangle / \pi) , \qquad (2.39)$$

with

$$\psi_{xA^{*}}^{(+)} = G_{x}(\chi_{b}^{(-)}\phi_{b}\phi_{x}\phi_{A^{*}} | V_{P} | \Phi_{aA}^{(+)}) + G_{x}(\chi_{b}^{(-)}\phi_{b}\phi_{x}\phi_{A^{*}} | V_{a} | \phi_{a}\phi_{A^{*}}) \times G_{a'}^{(+)}(\phi_{a}\phi_{A^{*}} | U_{a}' | \Phi_{aA}^{(+)}) .$$
(2.40)

The two terms on the rhs of Eq. (2.40) have originated from the elastic and inelastic components in (2.13), and describe, respectively, the Sim-IBF and Suc-IBF cross sections. Since the breakup reaction taking place in an inelastic channel is an EB in that channel, we can replace the interaction V_P by V_a , as we have done in obtaining the second term on the rhs of (2.40). This replacement should not be done, however, in the first term on the rhs of (2.40), i.e., in evaluating the Sim-IB and Sim-IBF amplitudes. The coupling term U'_a contained in V_P plays a crucial role here, as will be discussed in the next subsection.

E. Significance of using V_P

We shall begin this subsection by pointing out the crucial importance of having V_P (or sometimes its approximate V_a which is nothing but the interaction used in DWBA) rather than V, in the various cross section formulas we have derived above. Since $V_P = V - U_P$, to discuss the significance of the difference of having V or V_P is the same as to discuss the significance of subtracting U_P (or U_a) from V, in order to construct V_P (or V_a).

Let us first consider the case in which we set $V_P = V$, i.e., the case in which we have not subtracted U_P from V. Since this V operates upon the incident channel wave function, it can be replaced by VP and can be decomposed into $PVP + QVP = V_{PP} + V_{QP}$. By construction, P projects out only the scattering channels and thus V_{PP} is supposed to cause only the elastic and inelastic scattering, but no other types of reactions, including breakup. (The role which V_{QP} plays is completely opposite to this.) A very tricky aspect of the theory is the fact that, in spite of this property of V_{PP} , matrix elements such as

$$\langle \chi_b^{(-)} \chi_x^{(-)} \phi_b \phi_x \phi_A^* | V_{PP} | \Phi_{aA}^{(+)} \rangle$$
(2.41a)

do not vanish identically. Note that the ket state in (2.41a) is for the incident channel, while the bra state is for the breakup channel.

The reason why (2.41a) does not vanish identically is the so-called *nonorthogonality* of the wave functions of different channels. To see this more clearly, let us rewrite (2.41a) as

$$\sum_{a'} \langle \chi_b^{(-)} \chi_x^{(-)} \phi_b \phi_x \phi_A * | \widetilde{\chi}_{a'}^{(-)} \phi_a \phi_A * \rangle \\ \langle \chi_{a'}^{(-)} \phi_a \phi_A * | V_{PP} | \Phi_{aA}^{(+)} \rangle . \quad (2.41b)$$

The nonorthogonality of the channel wave functions reflects in the fact that the overlap integral, i.e., the first matrix element that appeared in (2.41b), has the property that

$$\langle \chi_a^{(-)} \chi_x^{(-)} \phi_b \phi_x \phi_A * | \tilde{\chi}_a^{(-)} \phi_a \phi_A \rangle \neq 0 .$$
 (2.41c)

This means that the state $\langle \chi_b^{(-)}\chi_x^{(-)}\phi_b\phi_x\phi_A |$, which is apparently for the breakup channel, *de facto* contains in it a component in which *b* and *x* have been recombined back into *a*. This component eventually results in the *a*-singles cross section, and is thus spurious (or unphysical) here, since it should not contribute to the *b*-singles cross section, which we are trying to calculate.

It is thus clear that our formalism must have a built-in recipe so as to eliminate these spurious components. The subtraction of U_P from V, so as to construct V_P as $V - U_P$, is precisely this recipe, as we shall show now.

Let us first retain only the leading term, i.e., only V_{PP} of (2.12) for U_P , postponing for the moment the consideration of the second term of (2.12). Since, as we explained above, we can replace V by $V_{PP} + V_{QP}$, we can evaluate $V_P = V - U_P$ as

$$V_P = V - U_P \simeq V - V_{PP} = V_{PP} + V_{QP} - V_{PP} = V_{QP} . \quad (2.42)$$

The significance of (2.42) is obvious. The V_P is now void of the troublesome part V_{PP} . Since a term like (2.41b), in which V_{PP} is replaced by V_{QP} , identically vanishes, there is no danger that that we retain in our calculation the nonorthogonality contributions, even if the inequality of (2.41c) remains valid.

Suppose now we approximate V_P by the DWBA interaction $V_a = V - U_a$. Equation (2.42) is then replaced by

$$V_a = (V_{PP} - U_a) + V_{OP} = U'_a + V_{OP} . \qquad (2.43)$$

Let us consider again a term like (2.41b), in which V_{PP} there is replaced by V_a of (2.43). Among the two terms U'_a and V_{QP} , the latter is the term that is responsible for producing the EB and Sim-IB amplitude. On the other hand, U'_a gives rise, when it appears in (2.41b), to an un-

physical contribution; it does so via the nonorthogonality of the breakup and inelastic-scattering channels, as seen again in (2.41c). This is why V_P , rather than V_a , must be used in the first term in (2.40) for Sim-IB.

Note that, because $\langle \phi_A | U'_a | \phi_A \rangle = 0$, U'_a does not give rise to any contribution to the EB amplitude. This is why the DWBA interaction V_a can be used in the last version of (2.38a), as well as in the second term in (2.40) for Suc-IB.

The above completes the explanation why the use of V_P (or V_a), rather than V, must be made in order to avoid unphysical contributions. In doing this, however, we have ignored the second term of (2.12), which we may call ΔV_{PP} for short. An important aspect of ΔV_{PP} is that it is complex. Thus, once ΔV_{PP} is retained, the exact cancellation between V_{PP} and U_P cannot be achieved. The imaginary part of U_P remains uncancelled.

Recall, however, the relation given above as (2.21). This relation states that $V_P = V - U_P$ eliminates exactly the unphysical (elastic and inelastic scattering) amplitudes from our starting formula (2.19). Note that (2.19) contained an exact Green's function G in it. The exact elimination embodied by (2.21) has, however, been lost, since we have made approximations, such as that seen in (2.22).

Once an approximation is done for G, however, it is more natural to modify V accordingly, so as to replace it by an "effective" interaction V^{eff} . A usual practice done in the direct reaction theory is to use a complex coupling potential for V^{eff} . When the IB and IBF reactions are calculated, we may use as V^{eff} , e.g., a sum of the optical potential between x and b and the individual nucleons in the target. When the EB and EBF reactions are calculated, a much simpler V^{eff} that is given as a sum of U_x and U_b may be used. (The justification of the use of $V^{\text{eff}} = U_x + U_b$ for the EB and EBF calculation has been given by IAV.¹⁷) When such an effective interaction is used, the cancellation between V_{PP} and U_P is expected to become sufficiently good, so that no significant amount of unphysical contributions remains in the calculations.

III. COMPARISON WITH OTHER THEORIES

Two recent papers, IAV (Ref. 17) and HM (Ref. 18), discussed the subject which is closely related to what we have discussed so far in the present paper. Since HM may be regarded as an approximate version of IAV, we shall discuss IAV in detail, and then comment briefly on HM.

We begin by remarking that, independent of the work of KM (Ref. 16) and UT (Ref. 11) which used the priorform formalism, Austern and Vincent (AV) (Ref. 22) had formulated the BF calculation by using the post-form formalism. Based on the AV formalism, Kasano and Ichimura (KI) (Ref. 23) then derived an explicit formula for the BF reaction, which may be written, as shown by Li, Udagawa, and Tamura (LUT),²⁴ as

$$\frac{d^2 \sigma^{\text{BF}}}{dE_b d\Omega_b} = (2\pi/\hbar w_a)\rho(E_b) \times \left[(\langle \psi_x^{(+)} | W_x | \psi_x^{(+)} \rangle + 2\operatorname{Re}\langle \psi_x^{(+)} | W_x | n \rangle + \langle n | W_x | n \rangle)/\pi \right], \qquad (3.1)$$

where

$$n \rangle = (\chi_b^{(-)} \phi_b \phi_x \phi_A \mid \Phi_{aA}^{(+)} \rangle .$$
(3.2)

Note that (3.1) consists of three terms, and that $\psi_x^{(+)}$ in (3.1) is the same as that given in (2.38a) (with $V = U_b + U_x$). This means that if it were not for the last two terms, (3.1) would agree with our EBF formula given in (2.37).

As seen, however, the extra two terms in (3.1) both depend on n of (3.2), and this n is nothing but the nonorthogonality overlap function (i.e., the projection of the elastic scattering wave function onto the b channel). As is well known, the appearance of this nonorthogonality term is due to the fact^{1,25} that the *first-order post-form* DWBA wave function inevitably includes in it the *lowest order* (elastic channel) wave function. As is also well known, the thus mixed up elastic component gives rise to an unphysical contribution when the first-order wave function is used in calculating two-step amplitudes. It is because of this that LUT argued that the terms in (3.1) involving n are unphysical and should not have been there.

IAV then responded to LUT in the following way. They first showed that (3.1) can be derived in the priorform formalism, as well in the post-form formalism of AV-KI. They then claimed that this became possible, because their formalism included the IB and IBF contributions; i.e., was not limited to the EB and EBF as it was the case in UT and hence in LUT. In other words, IVA claimed that the extra terms in (3.1) did represent the IB and IBF contributions, and thus were not unphysical.

It is true that the last two terms of (3.1) include, e.g., the IBF contributions, as we shall show below. However, we shall also show that they contain unphysical contributions as well.

The starting formula of IAV was the *b*-singles cross section given as,

$$\frac{d^2 \sigma_b^{\text{IAV}}}{dE_b d\Omega_b} = (2\pi/\hbar v_a) \rho(E_b) \sum_c |\langle \Phi_{b,c}^{(-)} | V_a | \Phi_{aA}^{(+)} \rangle|^2 .$$
(3.3)

The interaction V_a in (3.3) is the same as what we gave in (2.38a) [or (2.43)]. Also, $\Phi_{b,c}^{(-)}$ is the *d*-channel wave function defined as an eigenfunction of H'_d . We thus have

$$H'_{d}\Phi^{(-)}_{bc} = E_{bc}\Phi^{(-)}_{bc}, \qquad (3.4)$$

where, with our notation,

$$H'_d = H_x + K_b , \qquad (3.5a)$$

$$H_{x} = h_{A} + h_{x} + T_{xA} + V_{xA} . (3.5b)$$

It is important to note that H'_d differs from the *d*-channel optical model Hamiltonian that we used to define G_d in (2.23). H'_d has in it the interaction V_{xA} , while the Hamiltonian in our G_d had the optical potential U_x .

Since H'_d does not contain any interaction between b and x, the solution of (3.4) can be given as a product of eigenstates of H_x and K_b as

$$\Phi_{bc}^{(-)} = \chi_b^{(-)} \phi_b \Phi_{xA}^c , \qquad (3.6)$$

 Φ_{xA}^c satisfying

$$(E^{c} - H_{x})\Phi_{xA}^{c} = 0. (3.7)$$

We note here that, as is clear from (3.6), that the spectator approximation was also employed in IAV.

Equation (3.3) is a sum of prior-form DWBA breakup cross sections,¹⁷ each cross section being given as an absolute square of a breakup amplitude. To be emphasized here is the fact that these breakup amplitudes use the interaction V_a , rather than V_P . [Otherwise, (3.1) does not result from (3.3).] This fact and the discussion given in Sec. II E immediately lead us to the conclusion that (3.3) contains unphysical components. Since (3.1) is equivalent to (3.3), as proved by IAV, it can be concluded that (3.1) also contains unphysical components, and thus that our previous criticism²⁴ stands intact. The IAV work does not seem to have provided a valid justification of the AV-KI work.

Although the matter concerning Eqs. (3.1) and (3.3) thus appears rather clear, we may go here one step further and show explicitly that part of (3.3) is indeed a sum of inelastic cross sections.

This task can be done much easier (and it will suffice for our purpose) if we consider the integrated cross section, rather than the differential cross section. The task is made still easier, if we further assume that U_b in H'_d is real; then $\chi_b^{(-)}$ form a complete set. (This assumption also does not affect the conclusion on whether unphysical contributions vanish or not.) The completeness of $\chi_b^{(-)}$ being used, the integrated cross section in question is given as

$$\sigma_b^{\rm IAV} \equiv \int \frac{d^2 \sigma_b^{\rm IAV}}{dE_b d\Omega_b} dE_b d\Omega_b$$

= $(2\pi/\hbar v_a)(-\operatorname{Im}\langle \Phi_{aA}^{(+)} | V_a^{\dagger} G_d' V_a | \Phi_{aA}^{(+)} \rangle /\pi)$, (3.8)

where

$$G'_d = \frac{1}{E - H'_d + i\epsilon}$$
 (3.9)

We now use (2.43) for V_a . The $V_a^{\dagger}G'_dV_a$ factor in (3.8) can then be decomposed into four terms as

$$V_{a}^{\dagger}G_{d}'V_{a} = VQG_{d}'QV + U_{a}'^{\dagger}G_{d}'U_{a}' + VQG_{d}'U_{a}' + U_{a}'^{\dagger}G_{d}'QV .$$
(3.10)

From now on, we concentrate on the second term of (3.10), and note that the PG'_dP part of G'_d can be expressed as

$$PG'_{a}P(\equiv G_{a}^{\text{eff}}) = \frac{1}{E + \langle \phi_{a} | V_{xb} | \phi_{a} \rangle - h_{A} - T_{a} - U_{a}^{\text{eff}} + i\epsilon}$$
(3.11)

with

$$U_{a}^{\text{eff}} = \langle \phi_{a} \mid U_{b} + U_{x} \mid \phi_{a} \rangle + (H_{d})_{PQ} \frac{1}{E - (H_{d})_{QQ} + i\epsilon} (H_{d})_{QP} .$$
(3.12)

Equation (3.11), along with (3.12), is proved in Appendix B. What Eq. (3.11) shows is that $P_dG'_dP_d$ is an operator that describes propagation in the inelastic scattering channels.

Once PG'_dP is given as in (3.11), the contribution from the second term of (3.10) to σ_b^{IAV} can be obtained by repeating the procedure we followed in Sec. II D. The result is given as

$$\sum_{A^{*}} \int dE_{a}' d\Omega_{a} (2\pi/\hbar v_{a}) \rho(E_{a}') \left| \left\langle \Phi_{a'A^{*}}^{(-)}(E_{a}') \right| U_{a}' \left| \Phi_{aA}^{(+)} \right\rangle \right|^{2} + (2\pi/\hbar v_{a}) \left\{ \left\langle \Phi_{aA}^{(+)} \right| U_{a}'^{\dagger} G_{a}^{\text{eff}\dagger} \left[-\operatorname{Im}(U_{a}^{\text{eff}}) \right] G_{a}^{\text{eff}} U_{a}' \left| \Phi_{aA}^{(+)} \right\rangle / \pi \right\},$$
(3.13)

with

$$E'_{a} = E_{a} - (e_{A} * - e_{A}) + \langle \phi_{a} | V_{xb} | \phi_{a} \rangle . \qquad (3.14)$$

As is clear, the first term of (3.13) is a sum of pure inelastic scattering cross sections. On the other hand, the second term is a cross section for the fusion that takes place in the inelastic channels, thus including in it the Suc-IB and the Suc-IBF cross sections. In other words, (3.13) does include both physical and unphysical cross sections. [The physical part of the cross section in (3.13) has originated form the exact x-channel wave function Φ_{xA}^c in (3.3). Thus, it includes reactions taking place in the inelastic breakup channels.]

It is easy to see that the first term of (3.10) gives rise to the EB, EBF, Sim-IB, and Sim-IBF cross sections. Along with the Suc-IB and Suc-IBF cross sections, that can be extracted out of the second term in (3.13), these contributions taken together essentially reproduce what we obtained in Sec. II D.

The third and forth terms in (3.10) are interference terms and they have appeared, because IAV used the DWBA approximation so as to have G'_d in (3.7). Had this approximation been avoided, i.e., had the exact G appeared in (3.7), the resultant (3.10) should have been free from these interference terms. Because of this reason, we may regard the contributions from these interference terms to be unimportant, and can neglect them. (In any event, the integrands of various matrix elements appearing in these interference terms are expected to be highly oscillatory, and therefore these matrix elements will become small. Also, these matrix elements will have random phase, and thus cancel out among themselves.)

At this stage, we shall remark on the work of HM. It differs from IAV, in that it introduced one additional approximation beyond what IAV did, namely to neglect U_b in V_a . (HM emphasized that this approximation can be regarded as an extension of the spectator approximation normally made for the motion of b.) Because of this additional simplification, the HM cross section formula was much simpler than that of IAV. In fact the HM cross section is recognized as nothing but the third term of (3.1). Thus, the HM cross section is given as

$$\frac{d^2 \sigma_b^{\text{HM}}}{dE_b d\Omega_b} = (2\pi/\hbar v_a) \rho(E_b) (\langle n \mid W_x \mid n \rangle / \pi) . \quad (3.15)$$

We have already shown above that (3.15) contains unphysical inelastic scattering cross sections in it.

Both the IAV cross section of (3.1) and the HM cross

section (3.15) thus include inelastic cross sections. Since the inelastic cross sections are generally large, it is expected that the IAV cross section σ^{IAV} will be rather large. Note that we have already carried out²⁴ numerical evaluations of σ^{IAV} for a few example reactions, and compared the results with those for the UT-type cross section σ^{UT} . [In these calculations, we of course retained the imaginary part of U_b ; see the remark made just above Eq. (3.8).] It was found that, e.g., in the case of the ⁵⁸Ni(α ,p) reaction with E_{α} =80 and 160 MeV, the calculated σ^{IAV} was 10–100 times larger than was σ^{UT} . Since σ^{UT} agrees with experiment (at least for large E_P), it is clear that σ^{IAV} indeed seriously overpredicts the experimental cross sections.

The calculations made used the zero-range approximation. However, it has been found^{11-14,24} that the finiterange effects are often very important, particularly for the BF cross sections. Therefore, it is desirable to carry out finite-range calculations before making final conclusions concerning the magnitude of σ^{IAV} . Nevertheless, the results obtained in LUT seem to be consistent with our claim that σ^{IAV} includes large unphysical components.

Finally, we comment briefly on an additional controversy between IAV and ourselves. In the Appendix of LUT, we discussed the possibility that the AV formalism did not give a unique answer. We argued that an ambiguity is brought into the formalism when the on-theenergy-shell expression of the starting (post-form) formula of AV is transformed into the off-the-energy-shell expression [which is nothing but Eq. (3.1) of the present paper]. IAV then claimed (in its Appendix) that the argument of LUT was based on an approximation and that, if this approximation is suppressed, the ambiguity disappears. In terms of the notation of the present paper, the approximation made in LUT was to replace $G'_d G^{-1}_d$ by 1.

Without making this approximation, IAV repeated the calculation of the matrix element

$$\langle \rho^{(b)} | - \operatorname{Im}(E_x^{\dagger} - H_x)^{-1} | \rho^{(b)} \rangle$$

in (A6) of LUT, and obtained (A6') of IAV. As IAV stressed, (A6') does not contain in it the ambiguous term of LUT anymore, and we agree that LUT argument was indeed based on the above approximation. However, we now want to point out that (A6') still contains a term which turns out to be another source of ambiguity. The term in question is the expectation value of the kinetic energy operator with respect to n; i.e.,

(3.16)

$$|\alpha|^{2} \operatorname{Im} \langle n | T | n \rangle$$

= $|\alpha|^{2} (\hbar^{2}/2\mu_{x}) \frac{1}{2i} \int \left[n^{*} \frac{dn}{dr_{x}} - n \frac{dn^{*}}{dr_{x}} \right] dS$,

where α is an arbitrary number. If the integral in (3.16) vanishes, as IAV claimed, there is no ambiguity in their formalism. Their argument uses,²⁶ however, a convergence factor $[\exp(-\epsilon r_x)]$, discussed in Sec. III of IAV. It is true that (3.16) vanishes, if it is first evaluated at $r_x \gg 1/\epsilon$, and then the limit of $\epsilon \rightarrow 0$ is taken. However, if one sets $\epsilon=0$ from the beginning [or evaluates (3.16) at $r_x < 1/\epsilon$ and then takes the limit of $\epsilon \rightarrow 0$], one finds that (3.6) is nonvanishing. In other words, the integral of (3.16) is what one always encounters in evaluating the flux, we believe that it should consistently be evaluated by taking $\epsilon=0$. The term (3.16) is then nonvanishing so long as $|\alpha|^2 \neq 0$. This means that the ambiguity of the AV formalism which we discussed in LUT still remains.

IV. CONCLUDING REMARKS

The formulation of the BF calculations, presented earlier¹¹ for the elastic breakup-fusion (EBF) reaction, has been extended in Sec. II of the present paper, so as to include effects of target inelastic excitations, i.e., to calculate also the inelastic breakup-fusion (IBF) cross sections. Two types of inelastic excitations, i.e., the simultaneous and successive types, are considered. In the former, the target excitation takes place simultaneously with the breakup, while in the latter, the inelastic excitation takes place prior to the breakup. In formulating the IBF calculations, we took every care so as to prevent unphysical contributions from sneaking in, and explained in detail in Sec. II how we achieved this.

The formalism in the present paper (as well as that in Ref. 11) treats the breakup reaction as a transfer of a part of the projectile into the continuum of the target. As is well known, and as we explained in detail in Sec. II E, any transfer-type amplitude includes in it unphysical (elastic and inelastic scattering) components, if it is calculated in terms of DWBA, and by using the original interaction V. We then showed also in Sec. IIE that if this DWBA amplitude is calculated by using $V_a = V - U_a$, rather than V $(U_a$ is the optical potential in the incident channel), the unphysical contributions resulting from the elastic scattering are eliminated. The use of V_a thus makes it possible to calculate the EB and EBF amplitude correctly.^{11,15} Similarly, the use of V_P (where U_P is the extended optical model potential in that it includes the channel coupling terms) makes the IB and IBF amplitudes free from unphysical contributions.

We also discussed in Sec. III two recent papers; IAV (Ref. 17) and HM.¹⁸. We found that, although the IBF formula they derived did include correct IBF parts, they included unphysical contributions as well. (We traced the origin of this trouble to their use of V_a , rather than $V_{p.}$) Their formulas thus have a tendency to overestimate the cross sections significantly.

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APPENDIX A: PROOF OF EQ. (2.16)

Using (2.12) and (2.18), we can rewrite PV_P^{\dagger} as

$$PV_{P}^{\dagger} = P \left[V_{PP} + V_{PQ} - V_{PP} - V_{PQ} \frac{1}{E - H_{QQ} - i\epsilon} V_{QP} \right]$$
$$= PV_{PQ} \left[1 - \frac{1}{E - H_{QQ} - i\epsilon} V_{QP} \right].$$
(A1)

Inserting this and its conjugate into the rhs of (2.16), the latter can be rewritten as

$$PV_{P}^{\dagger}GV_{P}P = V_{PQ} \left[1 - \frac{1}{E - H_{QQ} - i\epsilon} V_{QP} \right] \frac{1}{E - H + i\epsilon} \times \left[1 - V_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} \right] V_{QP} . \quad (A2)$$

We next note that the following relation holds,

$$\begin{vmatrix} 1 - V_{PQ} \frac{1}{E - H_{QQ} + i\epsilon} \end{vmatrix}$$
$$= (E - H_{QQ} + i\epsilon - V_{PQ})Q \frac{1}{E - H_{QQ} + i\epsilon}$$
$$= (E - H + i\epsilon)Q \frac{1}{E - H_{QQ} + i\epsilon} .$$
(A3)

In going from the second to the third line in (A3), use was made of the fact that $(H_{PP} + H_{QP})Q = 0$. Now inserting (A3) into (A2), it is easy to see that the latter is reduced to the rhs of Eq. (2.16).

APPENDIX B: PROOF OF EQ. (3.11)

The proof of (3.11) along with (3.12) may be done as follows.^{17,20} We introduce first a state vector Z defined by

$$Z = G'_d P \rho , \qquad (B1)$$

where ρ is an arbitrary source function. The *P*- and *Q*-channel parts of *Z*, i.e., Z_P and Z_Q , respectively, then satisfy

$$[E - (H'_d)_{PP}]Z_P = P\rho + (H'_d)_{PQ}Z_Q , \qquad (B2a)$$

$$[E - (H'_d)_{OO}]Z_O = (H'_d)_{OP}Z_P .$$
(B2b)

We can solve (B2b) for Z_Q , and then insert it into (B2a). We then obtain,

$$\left| E - (H'_{d})_{PP} - (H'_{d})_{PQ} \frac{1}{E - (H'_{d})_{QQ} + i\epsilon} (H'_{d})_{QP} \right| Z_{P} = P\rho .$$
(B3)

The expression inside the bracket on the lhs of (B3) may

be rewritten as

$$E + \langle \phi_a | V_{xb} | \phi_a \rangle - h_A - T_a - U_a^{\text{eff}} , \qquad (B4)$$

by using U_a^{eff} which was defined in (3.12) of the text. If (B4) is used in (B3), Z_P is given as

$$Z_P = \frac{1}{E + \langle \phi_a | V_{xb} | \phi_a \rangle - h_A - T_a - U_a^{\text{eff}} + i\epsilon} P\rho . \quad (B5)$$

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Since ρ is arbitrary, the equivalence of (B5) to the *P*-channel part of (B1) results in the equality in (3.11). It is interesting to note that the energy E' $(=E + \langle \phi_a | V_{xb} | \phi_a \rangle)$ that appears in (3.11) differs from the original energy *E* by an expectation value of the potential energy of *a*. This has resulted simply because V_{xb} is neglected in G'_d . If V_{xb} is retained, E' is of course reduced back to the original energy *E*.

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