CROSS-SECTIONS FROM TDHF CALCULATIONS

E. A. Remler[†]
Department of Physics
College of William and Mary
Williamsburg, Virginia 23185

I. INTRODUCTION

This paper connects TDHF to reaction theory. Its approach differs that of previous related work[1,2] and leads to cross section formula which are free of some of their difficulties.

Arbitrarily many equivalent formula can be constructed relating exact solutions of the multiparticle Schroedinger equation to cross-sections. They are generally equivalent only in terms of exact solutions. Formula to be used with approximate solutions should not critically depend on properties of the exact solution poorly represented in the approximate one.

For example, scattering amplitudes are defined directly via the asymptotic values of exact wave functions. But since all presently known approximations for multiparticle wave functions fail asymptotically, this formula cannot be directly calculated. The usually used formula, of form $T_{fi} = \int \psi_f V_f \psi_i^{(+)}$, avoids this problem because it is insensitive to the asymptotic values of an approximate $\psi_i^{(+)}$. Another, of form $S_{fi} = (\psi_f^{(-)}, \psi_i^{(+)})$, similarly does not critically probe asymptotic values of $\psi_i^{(+)}$ or $\psi_f^{(-)}$. The manifestation of the analogous deficiency in TDHF is the appearance of the "spurious cross channel correlations". Analogs of both of the above formula, the first for inclusive and the second for exclusive cross sections, are used to circumvent this.

Another TDHF deficiency is its inability to describe the time evolution of a pure as opposed to a mixed state. Even though, neglecting dissipation, a TDHF solution can formally be put in the form of a wave function and, even if its initial Hartree-Fock (HF) states be considered reasonable approximate pure state wave packets, it seems unlikely that the putative wave function will retain much meaning after some time development. Clearly, without a wave function an S matrix cannot even be defined. This problem is circumvented by using analogs of the aforementioned formula in which density operators replace wave functions and as a result, the cross section replaces T_{fi} or S_{fi} respectively.

The next section begins by deriving a very general exact formula relating two body final state cross sections to density operators. Information from dynamics for a reaction A + B → C + D appears only in the form of density overlap, $\mathrm{tr}\rho_{CD}\rho_{AB}$, where $\rho_{AB}(\rho_{CD})$ is the density of the incoming (outgoing) channel at time $T_{AB}(-T_{CD})$. After a little manipulation, a simple and physically transparent formula is obtained.

[†]Work supported by the National Science Foundation under Grant Phy-80-06210

Two potentially serious problems however are associated with this formulation. The first arises from the fact that the trace is independent of T_{AB}-T_{CD} when exact densities are used but not after being approximated via TDHF.[8] A reasonable criterion is used to optimize its choice. The practical utility of this formula with respect to TDHF applications depends on its sensitivity to variations about the optimum choice of T_{AB}-T_{CD}. This remains to be investigated.[9]

Another problem arises from the fact that the formula requires a statistical averaging over two body final states. The theoretical uncertainty surrounding the very meaning of TDHF causes the relevant averaging functions to be similarly uncertain. Reasonable conjectures can be made and in addition, self consistency checks are available. Despite these problems the generality of the formula strongly suggests that if TDHF is at all applicable to such exclusive processes (an open question), it must be so in the form obtained here.

Section III treats inclusive cross sections for composite fragments - a measurement which should be more amenable to TDHF. The general approach has been described elsewhere[3] and has been applied to cascade[4] and hydrodynamic[5] models. Only points particular to TDHF applications are discussed here. Essentially none of the problems encountered in the previous section occur here.

Much of this paper can be generalized rather easily - Section II extended to more than two bodies, section III to more than one body. Both sections easily accommodate TDHF plus incoherent dissipation models. Certainly the basic formula used in section II and probably that used in section III can also serve in the context of mean field theory.

II. AVERAGED EXCLUSIVE CROSS-SECTIONS

Let $\phi = \underset{\sim}{r}, \underset{\sim}{k}$ denote a point in six dimensional phase space and $\rho_A(\phi_A)$ a density operator describing a mixture of eigenstates of nucleus A centered at ϕ_A. There are other parameters besides ϕ_A for ρ_A defining average values of internal energy, spin, etc., which are left implicit. This density is related to the density centered at the phase space origin by

$$\langle \underset{\sim}{k}_A'' | \rho_A(\phi_A) | \underset{\sim}{k}_A' \rangle = \exp(-i(\underset{\sim}{k}_A'' - \underset{\sim}{k}_A') \cdot \underset{\sim}{r}_A) \quad \langle \underset{\sim}{k}_A'' - \underset{\sim}{k}_A | \rho_A(0) | \underset{\sim}{k}_A' - \underset{\sim}{k}_A \rangle \quad . \tag{2.1}$$

The probability distribution function for A in state $\rho_A(\phi_A)$ is denoted by

$$g_A(\underset{\sim}{k}_A' - \underset{\sim}{k}_A) = \langle \underset{\sim}{k}_A' | \rho_A(\phi_A) | \underset{\sim}{k}_A' \rangle \tag{2.2}$$

and is assumed to be peaked at zero momentum and about the averages of its implicit arguments.

If $\rho_B(\phi_B)$ is similarly constructed for nucleus B and $\rho_{AB}(\phi_A,\phi_B)$ is the antisymmetrized direct product of ρ_A and ρ_B then as long as ϕ_A is sufficiently well separated from ϕ_B,

$$\langle \underset{\sim}{k}''_A, \underset{\sim}{k}''_B | \rho_{AB}(\phi_A,\phi_B) | \underset{\sim}{k}'_A, \underset{\sim}{k}'_B \rangle \cong \langle \underset{\sim}{k}''_A | \rho_A(\phi_A) | \underset{\sim}{k}'_A \rangle \langle \underset{\sim}{k}''_B | \rho_B(\phi_B) | \underset{\sim}{k}'_B \rangle \ . \tag{2.3}$$

Let $\rho_{AB}(\phi_A,\phi_B;T)$ be the exact density evolved after time T from $\rho_{AB}(\phi_A,\phi_B)$. For large enough T it will consist of well separated packets of collision products. Let C and D be two possible collision products in a two-nuclei final state and $\rho_{CD}(\phi_C,\phi_D)$ a density for them constructed as above. Then $\mathrm{tr}[\rho_{CD}(\phi_C,\phi_D)\rho_{AB}(\phi_A,\phi_B;T)]$ will be non-negligible only at well separated ϕ_C and ϕ_D. Using Eqs.(2.1-2.3) we obtain (h = 2π),

$$\int d\underset{\sim}{r}_C \, d\underset{\sim}{r}_D \, h^{-6} \, \mathrm{tr}[\rho_{CD}(\phi_C,\phi_D)\rho_{AB}(\phi_A,\phi_B;T)] =$$

$$\int d\underset{\sim}{k}'_C \, d\underset{\sim}{k}'_D \, g_C(\underset{\sim}{k}_C - \underset{\sim}{k}'_C) \, g_D(\underset{\sim}{k}_D - \underset{\sim}{k}'_D) \, \langle \underset{\sim}{k}'_C, \underset{\sim}{k}'_D | \rho_{AB}(\phi_A,\phi_B;T) | \underset{\sim}{k}'_C \ \underset{\sim}{k}'_D \rangle \ . \tag{2.4}$$

If ϕ_A and ϕ_B are well separated pre-collision configurations then the matrix element in Eq. (2.4) is just the resultant final state momentum distribution in the C + D channel. Integrating over impact parameter $\underset{\sim}{b}_B$ thus gives the averaged cross-section for beam nucleus B on target A;

$$\int d\underset{\sim}{b}_B \, d\underset{\sim}{r}_C \, d\underset{\sim}{r}_D \, h^{-6} \mathrm{tr}[\rho_{CD}(\phi_C,\phi_D)\rho_{AB}(\phi_A,\phi_B;T)] =$$

$$\int \prod_I d\underset{\sim}{k}'_I \ g_I(\underset{\sim}{k}_I - \underset{\sim}{k}'_I) \ \sigma(\underset{\sim}{k}'_C, \underset{\sim}{k}'_D ; \underset{\sim}{k}'_A, \underset{\sim}{k}'_B) \triangleq \bar{\sigma}(\underset{\sim}{k}_C, \underset{\sim}{k}_D ; \underset{\sim}{k}_A, \underset{\sim}{k}_B) \ , \tag{2.5}$$

where I = A,B,C,D, and σ is the momentum differential cross section for the reaction A + B → C + D and $\bar{\sigma}$ is the cross section averaged with g_I as weights. The averaging is implicitly over internal energy, nuclear spin, etc. The trace may be expressed more symmetrically by applying a time displacement to its argument;

$$\mathrm{tr}[\rho_{CD}(\phi_C,\phi_D)\rho_{AB}(\phi_A,\phi_B;T)] = \mathrm{tr}[\rho_{CD}(\phi_C,\phi_D;-T_{CD})\rho_{AB}(\phi_A,\phi_B;T_{AB})] \tag{2.6}$$

where in order for Eq. (2.5) to be valid we require $T_{AB} + T_{CD} = T >$ the time needed for A + B to collide starting from ϕ_A, ϕ_B and C + D to separate.

Our intent is to approximate this trace with the trace of corresponding density products formed from TDHF solutions. Thus let $\psi^{HF}_{AB}(\phi_A,\phi_B;t)$ be a TDHF solution evolved from the antisymmetrized product $A\psi^{HF}_A(\phi_A)\psi^{HF}_B(\phi_B) = \psi^{HF}_{AB}(\phi_A,\phi_B;0)$ of HF solutions centered at ϕ_A and ϕ_B. The corresponding density operator is $\rho^{HF}_{AB}(\phi_A,\phi_B;t) = \psi^{HF}_{AB}(\phi_A,\phi_B;t)\psi^{HF}_{AB}(\phi_A,\phi_B;t)^\dagger$. Defining a similar final state density ρ^{HF}_{CD}, we now assume that for appropriate values of the parameters $\phi_A, \ldots, \phi_D, T_{AB}$, T_{CD} to be discussed,

$$\mathrm{tr}\rho_{CD}\rho_{AB} \cong \mathrm{tr}\rho^{HF}_{CD}\rho^{HF}_{AB} \ . \tag{2.7}$$

Note that this does not require ψ^{HF}_{AB}, ψ^{HF}_{CD} to approximate exact time dependent wave functions of the system or ρ^{HF}_{AB}, ρ^{HF}_{CD}, exact time dependent densities, but only that the inner products defined in Eq. (2.7) be approximated. This seems to be the least one must ask of TDHF if it is to be applicable to two body final state cross sections. The approximate trace is given in terms of the determinant of the matrix *O* of over-

laps of initial and final state orbitals, $\psi^{HF}_{AB,i}$ and $\psi^{HF}_{CD,j}$ respectively, as follows.

$$O_{ji} = (\psi^{HF}_{CD,j}(\phi_C,\phi_D;-T_{CD}),\ \psi^{HF}_{AB,i}(\phi_A,\phi_B;T_{AB})) \tag{2.8}$$

$$\mathrm{tr}\rho^{HF}_{CD}\rho^{HF}_{AB} = |\mathrm{Det}\ O|^2 \quad . \tag{2.9}$$

The cross section formula developed so far

$$\bar{\sigma} \cong \int d\underset{\sim}{b}_B\ d\underset{\sim}{r}_C\ d\underset{\sim}{r}_D\ h^{-6}\mathrm{tr}\rho^{HF}_{CD}\rho^{HF}_{AB} \tag{2.10}$$

with $\bar{\sigma}$ given by Eq. (2.5) and the trace by Eqs. (2.8) and (2.9) is an almost necessary consequence of the (albeit perhaps overly optimistic) assumption that TDHF has any relevance to such averaged exclusive cross sections. Two major questions however remain. (1) What are $g_A \ldots g_D$. (2) What to use for T_{AB} and T_{CD}. The answers to these, in contrast, are not so well determined.

There is virtually no theory available on which to base an answer to the first question. A "maximalist" opinion of the meaning of TDHF might be that if ψ^{HF}_I are e.g. HF ground state wave functions then the g_I average only over three momentum and total spin projection. Their form is then given by the calculable total momentum and spin distribution in a HF packet. A similar statement would hold for transitions to excited states.

But this is not necessarily true. The g_I might average also over many nuclear eigenstates of internal energy. Their shape in this case is unknown. One can hope and might reasonably expect that their internal energy distribution is obtainable by simple statistical arguments or that experiment is insensitive to it, or both. After discussion of the second question we shall see that some theoretical experiments may shed light on their shape.

We turn now to the division of T into T_{AB} and T_{CD}. It should be chosen to minimize the error in Eq. (2.7). For this question some simple intuitive arguments are available.

We are free to choose for simplicity $\underset{\sim}{r}_A = (\underset{\sim}{0}, Z_A)$, $\underset{\sim}{r}_B = (\underset{\sim}{b}_B, Z_B)$ so that $|Z_A - Z_B|$ is the minimum initial distance between target A and projectile B. Clearly this must be chosen to be sufficiently greater than the entrance channel interaction's range R_{AB}. Let the initial velocities be $\underset{\sim}{v}_A = \underset{\sim}{k}_A/M_A = (0,v_A)$ and $\underset{\sim}{v}_B = \underset{\sim}{k}_B/M_B = (\underset{\sim}{0}, -v_B)$ where v_A and v_B are their magnitudes. For a pre-collision configuration this requires $Z_A < 0$, $Z_B > 0$. If in addition we set $Z_A/v_A + Z_B/v_B = 0$, then non-interacting nuclei would achieve closest approach after a time $|Z_A/v_A| = Z_B/v_B$. About this time ρ^{HF}_{AB} will typically be most dense and begin to generate outgoing components. After this time any meaningfulness of ρ^{HF}_{AB} may be expected to deteriorate rapidly as ρ_{AB} begins to develop distinct final state channels which ρ^{HF}_{AB} cannot describe.

Consider the choice of this time for T_{AB}. Then $|\mathrm{Det}\ O|$ will be non-negligible only for post-collision configurations ϕ_C, ϕ_D which, projected backwards in time by T_{CD}, describe a coalescent system near that of A + B at T_{AB}. What ϕ_C, ϕ_D

do this? Consider first the case in which $\underset{\sim}{v}_C$ and $\underset{\sim}{v}_D$ are colinear and oppositely directed. Then their projected positions $Z_C = \underset{\sim}{r}_C \cdot \underset{\sim}{v}_C / v_C$, $Z_D = \underset{\sim}{r}_D \cdot \underset{\sim}{v}_C / v_C = -\underset{\sim}{r}_D \cdot \underset{\sim}{v}_D / v_D$ should satisfy $Z_C/v_C \cong |Z_D|/v_D \cong T_{CD}$. Large enough T_{CD} therefore guarantees a separation $|Z_C - Z_D|$ sufficiently larger than the final channel interaction range R_{CD}. We can always adjust T and $|Z_A - Z_B|$ so that $T_{AB} = T_{CD} = \frac{1}{2}T$.

Each HF packet translates itself with unchanging shape when isolated. Thus for large enough $|Z_C - Z_D|$

$$\rho^{HF}_{CD}(\underset{\sim}{r}_C, \underset{\sim}{k}_C, \underset{\sim}{r}_D, \underset{\sim}{k}_D; -\tfrac{1}{2}T + \tau) = \rho^{HF}_{CD}(\underset{\sim}{r}_C + \underset{\sim}{v}_C\tau, \underset{\sim}{k}_C, \underset{\sim}{r}_D + \underset{\sim}{v}_D\tau, \underset{\sim}{k}_D; -\tfrac{1}{2}T) \tag{2.11}$$

with a similar expression for ρ^{HF}_{AB}. This is the analog of the "intertwining relation" in ordinary scattering theory. This allows a spatial displacement to be converted to a time displacement as follows. Let $\underset{\sim}{b}_C$ and $\underset{\sim}{b}_D$ be impact parameter type two-vectors perpendicular to the respective $\underset{\sim}{v}_C$ and $\underset{\sim}{v}_D$ and let

$$\lambda = (\underset{\sim}{r}_C \cdot \underset{\sim}{v}_C + \underset{\sim}{r}_D \cdot \underset{\sim}{v}_D)/v_{CD}$$

$$\eta = (\underset{\sim}{r}_C \cdot \underset{\sim}{v}_D - \underset{\sim}{r}_D \cdot \underset{\sim}{v}_C)/v_{CD}$$

$$v_{CD} = (v_C^2 + v_D^2)^{1/2} \tag{2.12}$$

Considering $\underset{\sim}{r}_C$ and $\underset{\sim}{r}_D$ as functions of $\underset{\sim}{b}_C, \underset{\sim}{b}_D, \lambda, \eta$ the intertwining relation allows us to write Eq. (2.10) in the form

$$\bar{\sigma} = v_{CD} h^{-6} \int d\underset{\sim}{b}_B d\underset{\sim}{b}_C d\underset{\sim}{b}_D d\eta d\tau \times \mathrm{tr} \rho^{HF}_{CD}(\phi_C, \phi_D; -\tfrac{1}{2}T + \tau) \rho^{HF}_{AB}(\phi_A, \phi_B; \tfrac{1}{2}T) \tag{2.13}$$

The spatial integral for C and D is now over a five dimensional hyperplane $\lambda = \frac{1}{2}v_{CD}T$. The integral for B is over the two dimensional impact parameter hyperplane $Z_B = \frac{1}{2}v_B T$ with $\underset{\sim}{r}_A$ fixed at $(\underset{\sim}{0}, -\frac{1}{2}\underset{\sim}{v}_A T)$ so that the λ parameter for the pre-collision configuration is

$$(\underset{\sim}{r}_A \cdot \underset{\sim}{v}_A + \underset{\sim}{r}_B \cdot \underset{\sim}{v}_B)/v_{AB} = -\tfrac{1}{2}Tv_{AB} \quad . \tag{2.14}$$

The λ hyperplane for C and D was chosen so that freely travelling nuclei would reach it in a time $\frac{1}{2}T$ from their point of closest approach. Thus we expect the integrand in Eq. (2.13) to be maximum somewhere around $\tau = 0$ and $\eta = \underset{\sim}{b}_C = \underset{\sim}{b}_D = 0$. The nuclear separation at this point is $|Z_C - Z_D| = \frac{1}{2}T(v_C + v_D)$. Thus T must be chosen sufficiently greater than both $R_{AB}/\frac{1}{2}(v_A + v_B)$ and $R_{CD}/\frac{1}{2}(v_C + v_D)$ but is otherwise arbitrary. Having picked such a T, all the remaining hyperplane parameters Z_A, Z_B, λ are determined as indicated in terms of it.

Recall now that the choice of a fixed T_{AB} was somewhat arbitrary and has resulted in an expression, Eq. (2.13), which is asymmetric between AB and CD within the trace. That expression uses $\tau < 0$ values where ρ^{HF}_{CD} is in its rapidly deteriorating range of validity. The total error in the trace can be minimized when the error in ρ^{HF}_{AB} and ρ^{HF}_{CD} is equalized. This can be done by changing T_{AB} so that it is λ (or τ) dependent while keeping T fixed. Since to lowest order the error will vary

linearly in τ, on the average we can expect to improve accuracy by replacing $T_{AB} \to \frac{1}{2}T - \frac{1}{2}\tau$, $T_{CD} \to -\frac{1}{2}T + \frac{1}{2}\tau$ in Eq. (2.13):

$$\bar{\sigma} = v_{CD}\, h^{-6} \int d\underset{\sim}{b}_B d\underset{\sim}{b}_C d\underset{\sim}{b}_D d\eta d\tau$$

$$\times \left|\mathrm{Det}(\psi^{HF}_{CD,j}(\phi_C,\phi_D;\ -\tfrac{1}{2}(T-\tau)),\ \psi^{HF}_{AB,i}(\phi_A,\phi_B;\ +\tfrac{1}{2}(T-\tau)))\right|^2 \quad . \tag{2.15}$$

Note that the integrand of this 8 dimensional integral should be smoothly peaked about the zero of its arguments. No oscillations are generally expected. Therefore it should be approximable by numerical interpolation techniques using relatively few grid points.

We must finally address the question of the choice of $\underset{\sim}{v}_C$ and $\underset{\sim}{v}_D$. Recall they were arbitrarily taken to be opposite and collinear. In fact the integral determining $\bar{\sigma}$ in Eq. (2.5) can be done for arbitrary $\underset{\sim}{k}_C$ and $\underset{\sim}{k}_D$. Consider center of mass scattering and the "maximalist" interpretation of the meaning of the TDHF solutions. In this case a choice of $\underset{\sim}{k}_A \ldots \underset{\sim}{k}_D$ which satisfies four momentum conservation will agree with that made in the preceding discussion. Assuming the transition matrix is relatively slowly varying we can write (neglecting spin factors)

$$\sigma(\underset{\sim}{k}_C,\underset{\sim}{k}_D;\underset{\sim}{k}_A,\underset{\sim}{k}_B) \triangleq \Gamma(\underset{\sim}{k}_C\underset{\sim}{k}_D;\underset{\sim}{k}_A\underset{\sim}{k}_B)\delta^4(k_C+k_D-k_A-k_B) \tag{2.16}$$

$$\bar{\sigma} \cong \Gamma \int \prod_i d\underset{\sim}{k}'_I g_I(\underset{\sim}{k}'_I-\underset{\sim}{k}_I)\delta^4(k_C+k_D-k_A-k_B) \tag{2.17}$$

With the "maximalist" interpretation, g_I are known and the behavior of $\bar{\sigma}$ as $\underset{\sim}{k}_I$ vary near the 4 momentum shell can be computed by Eq. (2.17) and compared to the computed integral in Eq. (2.15). This is a self consistency check. Without the maximalist interpretation such a comparison provides information which may be used to empirically determine the form of the g_I. This point requires further investigation and may lead to some insight into the meaning of the TDHF approximation.

III. INCLUSIVE CROSS-SECTIONS

If, as before, a TDHF solution is written as $\psi^{HF}_{AB}(\phi_A\phi_B;t)$, then the number density of nucleons can be written as $(\psi^{HF}_{AB},\hat{\psi}^\dagger_{\underset{\sim}{k}}\hat{\psi}_{\underset{\sim}{k}}\psi^{HF}_{AB})$ where $\hat{\psi}_{\underset{\sim}{k}}$ denotes a momentum $\underset{\sim}{k}$ annihilation operator. Clearly, this expression does not distinguish asymptotically bound from free nucleons. To emphasize this we call this number density, primordial. Assuming ϕ_A,ϕ_B corresponds to a well separated initial state configuration, the limit of the primordial nucleon number density as $t \to \infty$ is denoted as $\tilde{\sigma}(\underset{\sim}{k};\phi_A\phi_B)$ and is called the primordial inclusive nucleon cross-section (for initial state ϕ_A,ϕ_B). The usual cross-section for asymptotically free nucleons is written without a tilde. The difference between these is the cross-section for bound ("virtual") nucleons;

$$\tilde{\sigma}(\underset{\sim}{k};\phi_A\phi_B) = \sigma(\underset{\sim}{k};\phi_A\phi_B) + \sigma^{(v)}(\underset{\sim}{k};\phi_A\phi_B) \quad . \tag{3.1}$$

The expression for $\tilde{\sigma}$ can be generalized by writing it in terms of the density operator. Thus

$$\tilde{\sigma}(\underset{\sim}{k};\phi_A\phi_B) = \lim_{t\to\infty} tr[\hat{\psi}^\dagger_{\underset{\sim}{k}}\hat{\psi}_{\underset{\sim}{k}}\rho_{AB}(\phi_A,\phi_B;t)] \quad . \tag{3.2}$$

When ρ_{AB} is exact, so is $\tilde{\sigma}$. Use of ρ^{HF}_{AB} gives an approximate $\tilde{\sigma}$. Equation (3.2) can also be used with generalizations of TDHF which include incoherent ("two body collision") terms where ρ^{HF}_{AB} but not ψ^{HF}_{AB} has meaning.

It will be useful to consider an alternate form of Eq. (3.2); leaving ϕ_A, ϕ_B, A, B implicit, we can write

$$\Delta\tilde{\sigma}(\underset{\sim}{k}) = \int_0^\infty \partial_t tr[\hat{\psi}^\dagger_{\underset{\sim}{k}}\hat{\psi}_{\underset{\sim}{k}}\rho(t)]dt = \int_0^\infty tr([i\hat{H},\hat{\psi}^\dagger_{\underset{\sim}{k}}\psi_{\underset{\sim}{k}}]\rho(t))dt = \int_0^\infty tr([i\hat{V},\hat{\psi}^\dagger_{\underset{\sim}{k}}\hat{\psi}_{\underset{\sim}{k}}]\rho(t))dt \ , \tag{3.3}$$

$$\Delta\tilde{\sigma}(\underset{\sim}{k}) \triangleq \tilde{\sigma}(\underset{\sim}{k}) - tr[\hat{\psi}^\dagger_{\underset{\sim}{k}}\psi_{\underset{\sim}{k}}\rho(0)] \ , \tag{3.4}$$

where $\hat{H}$ is the Hamiltonian and $\hat{V}$ is the potential

$$\hat{V} = \tfrac{1}{4}\int d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 d\underset{\sim}{k}'_1 d\underset{\sim}{k}'_2 \hat{\psi}^\dagger_{\underset{\sim}{k}'_2}\hat{\psi}^\dagger_{\underset{\sim}{k}'_1}\langle \underset{\sim}{k}'_1\underset{\sim}{k}'_2|V|\underset{\sim}{k}_2\underset{\sim}{k}_1\rangle\hat{\psi}_{\underset{\sim}{k}_1}\hat{\psi}_{\underset{\sim}{k}_2} \tag{3.5}$$

Consider the effect of approximating ρ by ρ^{HF} in Eq. (3.3). If ρ^{HF} is of thermal Hartree-Fock[6,7] form then

$$tr(\hat{\psi}^\dagger_{\underset{\sim}{k}'_N}\cdots\hat{\psi}^\dagger_{\underset{\sim}{k}'_1}\hat{\psi}_{\underset{\sim}{k}_1}\cdots\hat{\psi}_{\underset{\sim}{k}_N}\rho^{HF}) \triangleq \langle \underset{\sim}{k}_N\cdots\underset{\sim}{k}_1|n^{(N)}|\underset{\sim}{k}'_1\cdots\underset{\sim}{k}'_N\rangle = Det\langle \underset{\sim}{k}_i|n|\underset{\sim}{k}'_j\rangle \quad , \tag{3.6}$$

$$\langle \underset{\sim}{k}'|n|\underset{\sim}{k}\rangle \triangleq tr[\hat{\psi}^\dagger_{\underset{\sim}{k}}\hat{\psi}_{\underset{\sim}{k}},\rho^{HF}] \tag{3.7}$$

This rule includes the case $\rho^{HF}_{AB} = \psi_{AB}\psi^\dagger_{AB}$. Under this assumption, Eq. (3.5) into Eq. (3.3) yields

$$\Delta\tilde{\sigma}(\underset{\sim}{k}) = \int_0^\infty \langle \underset{\sim}{k}|[n,iv]|\underset{\sim}{k}\rangle dt \tag{3.8}$$

where v is a mean field potential

$$\langle \underset{\sim}{k}'|v|\underset{\sim}{k}\rangle = \int d\underset{\sim}{p}d\underset{\sim}{p}'\langle \underset{\sim}{p}'\underset{\sim}{k}'|V|\underset{\sim}{k}\underset{\sim}{p}\rangle\langle p|n|p'\rangle \tag{3.9}$$

This result suggests that V should be replaced by the effective (e.g. G-matrix) interaction whenever ρ is approximated by ρ^{HF}. This turns v into the TDHF potential and if n is the TDHF generated number density, Eq. (3.8) implies

$$\Delta\tilde{\sigma}(\underset{\sim}{k}) = \int_0^\infty \langle \underset{\sim}{k}|[-ih,n]\underset{\sim}{k}\rangle dt = \int_0^\infty \langle \underset{\sim}{k}|\partial_t n|\underset{\sim}{k}\rangle dt \tag{3.10}$$

where h is the TDHF Hamiltonian. This is exactly the expected result.

We are now prepared to generalize the preceding to composite fragment production. The generalization of Eq. (3.2) is

$$\tilde{\sigma}_C(\underset{\sim}{k};\phi_A\phi_B) = \lim_{t\to\infty} tr(\hat{\psi}^\dagger_{C,\underset{\sim}{k}}\hat{\psi}_{C,\underset{\sim}{k}}\rho_{AB}(\phi_A,\phi_B;t)) \tag{3.11}$$

where $\hat{\psi}_{C,\underset{\sim}{k}}$ annihilates a composite C of momentum $\underset{\sim}{k}$;

$$\hat{\psi}_{C,\underset{\sim}{k}} \triangleq \int d\underset{\sim}{k}_1\cdots d\underset{\sim}{k}_N \langle C,\underset{\sim}{k}|\underset{\sim}{k}_1\cdots\underset{\sim}{k}_N\rangle/N! \quad \hat{\psi}_{\underset{\sim}{k}_N}\cdots\hat{\psi}_{\underset{\sim}{k}_1} \tag{3.12}$$

Similarly, Eq. (3.1) suitably generalized still hold;[3] $\tilde{\sigma}_C$ includes contributions from virtual C's in larger composites which must be subtracted out to obtain the true inclusive cross-section σ_C.

As with Eq. (3.3), we re-express Eq. (3.11) as a difference,

$$\Delta\tilde{\sigma}_C(\underset{\sim}{k}) = \int_0^\infty \mathrm{tr}([i\hat{H},\hat{\psi}^\dagger_{C,\underset{\sim}{k}}\hat{\psi}_{C,\underset{\sim}{k}}]\rho(t))\,dt \quad . \tag{3.13}$$

After some algebra, the generalization of the last step in Eq. (3.3) is found to be

$$\Delta\tilde{\sigma}_C(\underset{\sim}{k}) = \int_0^\infty \mathrm{tr}(:[i\hat{V},\hat{\psi}^\dagger_{C,\underset{\sim}{k}}\hat{\psi}_{C,\underset{\sim}{k}}]:\rho(t))dt \tag{3.14}$$

where colons denote normal ordering. This form contains the information that $\hat{\psi}_{C,\underset{\sim}{k}}$ annihilates an exact eigenstate of $\hat{H}$.

As before we may now approximate ρ by ρ^{HF} and replace V by the effective interaction. Using Eq. (3.6) and some further algebra, we can write the result as

$$\Delta\tilde{\sigma}_C(\underset{\sim}{k}) = \int_0^\infty \langle C,\underset{\sim}{k}|[n^{(N)},i(v-V')]|\underset{\sim}{k},C\rangle/(N!)^2 dt \quad . \tag{3.15}$$

The notation is now as follows: The ket $|\underset{\sim}{k},C\rangle$ has components $\langle \underset{\sim}{k}_1\ldots\underset{\sim}{k}_N|\underset{\sim}{k},C\rangle$ as defined by Eq. (3.12) and is antisymmetric in $\underset{\sim}{k}_1\ldots\underset{\sim}{k}_N$. The matrix $n^{(N)}$ is defined by Eq. (3.6). The matrix v is now a sum of N(TDHF) potentials each defined as in Eq. (3.9), each operating on a separate momentum. The matrix V' is a sum over $\frac{1}{2}N(N-1)$ two body operators, one for each distinct pair of momenta $V' = \sum_{i<j} V'_{ij}$,

$$\langle \underset{\sim}{k}'_i\underset{\sim}{k}'_j|V'_{ij}|\underset{\sim}{k}_j\underset{\sim}{k}_i\rangle = \int d\underset{\sim}{q}_j\, d\underset{\sim}{q}'_j \langle \underset{\sim}{k}'_j|n|\underset{\sim}{q}'_j\rangle\langle \underset{\sim}{k}'_i\underset{\sim}{q}'_j|V_{ij}|\underset{\sim}{q}_j\underset{\sim}{k}_i\rangle\langle \underset{\sim}{q}_j|n|\underset{\sim}{k}_j\rangle \quad , \tag{3.16}$$

To obtain Eq. (3.15) the pure state condition $n^2 = n$ has been used. Thus n is a projection and $[n^{(N)},iV']$ can be considered as the time rate of change of $n^{(N)}$ due to interactions between fragment constituents. The fact that V' is subtracted in Eq. (3.15) shows that fragment production is determined by the potential felt by fragment constituents due to particles exterior to the fragment. This is exactly what one expects on the basis of multiparticle scattering theory.[3]

Since $h_0 + v$ generates the time rate of change in $n^{(N)}$,

$$\int_0^\infty \langle C,\underset{\sim}{k}|[n^{(N)},iv]|\underset{\sim}{k},C\rangle dt = \int_0^\infty \langle C,\underset{\sim}{k}|\partial_t n^{(N)} - [n^{(N)},ih_0]|\underset{\sim}{k},C\rangle\, dt \quad . \tag{3.17}$$

Assuming $\lim_{t\to\infty} \langle C,\underset{\sim}{k}|n^{(N)}|\underset{\sim}{k},C\rangle = 0$, we find

$$\tilde{\sigma}_C(\underset{\sim}{k}) = \int_0^\infty \langle C,\underset{\sim}{k}|[n^{(N)},-ih']|\underset{\sim}{k},C\rangle/(N!)^2 dt \tag{3.18}$$

where $h' = h_0 + V'$. For purposes of computation one might calculate a virtual change in $|\underset{\sim}{k},C\rangle$ over a time segment dt by

$$\delta'_t|\underset{\sim}{k},C\rangle = -ih'|\underset{\sim}{k},C\rangle dt \quad . \tag{3.19}$$

Letting t become a time segment index, Eq. (3.18) becomes

$$\tilde{\sigma}_C(\underset{\sim}{k}) = \sum_t \delta'_t \langle C,\underset{\sim}{k}|n^{(N)}|\underset{\sim}{k},C\rangle/(N!)^2 \tag{3.20}$$

Noting that $n^{(N)}$ is the sum of N! terms each of which contributes the same we get finally

$$\tilde{\sigma}_C(\underset{\sim}{k}) = \sum_t \delta'_t \sum_{(\alpha_1\ldots\alpha_N)} |\langle \alpha_N\ldots\alpha_1|\underset{\sim}{k},C\rangle|^2 \tag{3.21}$$

where we have used the fact that

$$n = \sum_{\alpha} |\alpha\rangle\langle\alpha| \tag{3.22}$$

each $|\alpha\rangle = \psi_{\alpha}(\phi_A, \phi_B; t)$, being an orbital at time interval t. The sum over $(\alpha_1 \ldots \alpha_N)$ extends over all sets of N (out of $N_A + N_B$) orbitals which do not differ by a permutation amongst themselves.

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8. If mean field theory is used here instead of TDHF this problem does not arise.
9. Note however that the trace does not oscillate as in the analogous case discussed in Reference 1.