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Two-tier formulation of multichannel scattering theory and hypervirial theorems

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Abstract

Complex dynamics of a multichannel scattering may be treated by a variational procedure. But the conventional variational principles are not readily applicable because of (i) the intrinsic difficulties of unstable fluctuations in the calculated amplitudes as functions of nonlinear parameters and (ii) lack of criteria to optimize the solutions. A two-tier theory is formulated in which the complex dynamical mixing and the asymptotic channel sector are treated separately, but as a coupled system, such that the instability problem (i) is resolved naturally in a mathematically consistent way, even when most of the weakly coupled open channels are neglected. The resulting solution is stable, but not necessarily optimal. Modified forms of hypervirial theorems are introduced to optimize the solutions, thus rectifying the shortcoming (ii). Thus, the reformulated theory for the scattering states, coupled with a properly chosen hypervirial theorem, can be applied effectively to many-body, multichannel scattering systems.

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1. Introduction

Analyses of a many-body system with more than two active particles require drastic approximations. Whether an exact Hamiltonian of the system is known or a model Hamiltonian is being studied, it is important that approximate solutions one obtains are reliable. The current computational capability is such that any two-body scattering systems are numerically solvable, essentially exactly. But for systems with three or more active particles, and with more than two clusters as in a breakup, reliable solutions are not always readily obtainable. The formulation in this paper should be especially relevant to analysing many-body scattering systems with many open channels, including the breakup reactions but for practical reasons not all of which can be explicitly included.

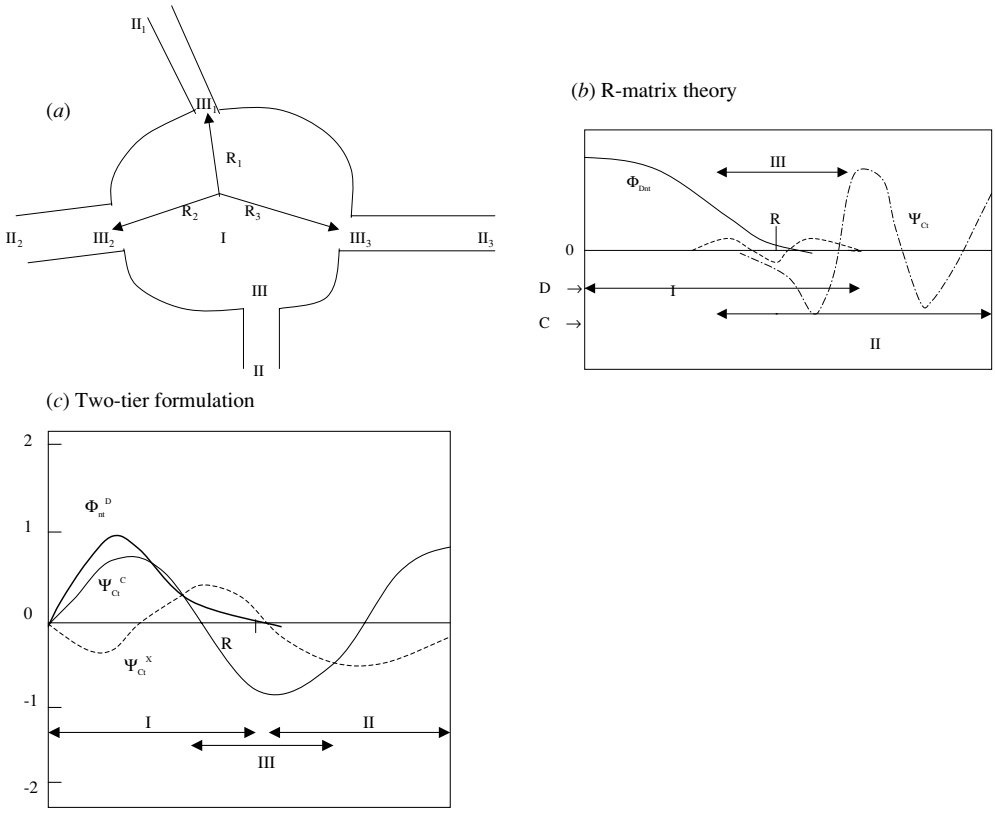

Figure 1. (1) The three regions of configuration space are indicated; the inner interaction region I, the asymptotic region III and the matching region II. The boundaries between the regions are generally not sharp, but the range R may be roughly defined that separates the different regions. It may be different for each individual channel. (2) The R-matrix picture of the trial functions. Construction of the variational trial functions are indicated to be localized, such that nearly zero overlap between the functions in the I and III regions. The connection between these two regions is made through $\Psi_{\mathrm{I}it}$, so that chance of singular roots of the M matrix is eliminated when $\Psi_{\mathrm{P}t}$ is treated variationally. (3) The structure of the trial functions is different for the two-tier approach, as compared to that in (2).

The variational principles (VP) have been used with great efficiency in treating many-body bound systems, mainly because of the powerful Ritz extremum principle (Ritz 1908, Rayleigh 1937) that can guide the solution in terms of the boundedness of the system energy spectrum. It is a minimim principle in that the calculated ground-state energy, for example, is not only a stationary value but also a bound on the exact energy E_0, although the latter is not known *a priori*. Therefore, the solution can be systematically improved. This bound property is a direct consequence of the fact that the shifted Hamiltonian $M_0 = H - E_0$ is positive definite, $M_0 \geqslant 0$, for the ground-state energy E_0. An equally powerful approach for excited bound states also exists in the form of Hylleraas–Undheim theorem (Hylleraas and Undheim 1930, MacDonald 1933).

The variational principles were then proposed (Hulthen 1944, 1948, Kohn 1948, Schwinger 1950) for the scattering states, although the mathematical properties are quite different. In fact, the VP are uniquely effective in treating the strongly interacting region, as in the zone I of figure 1(*a*), where the complex dynamical mixing among the channels takes

place, but the presence of the channel region II, with the scattering wavefunctions which are not square-integrable, totally changes the situation. The channel region usually involves a few clusters in continua, and its wavefunction contains all the asymptotic boundary conditions which are pre-assigned, that include all the internal cluster functions specified. The matching in region III of the solutions of regions I and II then provides the scattering amplitudes. The VP for scattering states generally lack the crucial and useful properties of the bounded spectrum. That is, the total scattering energy E is embedded in the spectrum of H such that $M = H - E$ can assume either sign, and thus in the error term. This has been the source of intrinsic difficulties which have retarded their applications for many years: (i) unstable fluctuations in the calculated amplitudes (Schwartz 1961a, 1961b, Wu and Ohmura 1962) as the nonlinear parameters in the trial functions are varied, and (ii) there are no built-in criteria to guide the solution to the correct value. Evidently, the shortcomings (i) and (ii) are the direct result of the fact that the spectrum of the operator M is *not* positive definite in the case of scattering.

However, progress has been made in later years in deriving the approaches with the bound properties for zero energy scattering (Spruch and Rosenberg 1960), and for low energy scattering (Hahn and Spruch 1967) with a few open channels, where difficulties (i) and (ii) were simultaneously removed. Specifically in the latter approach, the original spectrum of M is divided into two parts, as summarized in the appendix, such that the resulting 'closed channel' operator M^Q satisfies the inequality $M^Q \geqslant 0$ for non-zero scattering energy. It is a rigorous minimum principle, provided that *all the open channels at a given E are separated* from M^Q and *are treated exactly numerically.* But the required procedure to maintain the bound property is often too rigid and cumbersome for ready applications. Although the complex closed channel component in region I of figure 1(*a*) is still treated variationally, the necessary projection operators to separate the spectrum into two parts are difficult to derive. In fact, the requirement for the projection operators has been removed later in a generalized variational bounds formulation (Hahn 1969, 1970), so that the minimum principle can be applied to general multichannel scattering, as long as the number of open channels is not large.

The approaches with bounded M^Q break down as the scattering energy E increases and the number of open channels becomes very large, as in a breakup, such that, mainly for practical reasons, a large part of the open channels has to be omitted. Almost all the theoretical procedures available retain only some of the strongly coupled channels. Consequently, the all-important bound properties of M^Q are lost, and the methods which depend exclusively on the boundedness of a modified (closed channel) energy spectrum for their validity are no longer applicable. In this paper, we consider the scattering theory which does *not* require the full inclusion of *all* the open channels for its validity.

Truncation of any part of open channels is an approximation, which can only be justified *a posteriori* if the coupling to the neglected channels is weak. The bound principle is thus lost, but the theory to be developed below does not depend on it.

The conventional VP for scattering are reviewed in section 2, and the difficulty (i) of unstable fluctuation of the calculated amplitudes is illustrated. A new two-tier approach is presented in section 3, which automatically removes the difficulty (i). A flow chart is provided in figure 2 for clarity. Section 4 contains a series of hypervirial theorems which may be used to test the variational solutions, thus remedying the difficulty (ii).

2. The conventional VP for scattering states and the instability difficulty

We first briefly review the original VP for scattering states and discuss the difficulties (i) and (ii) mentioned in the previous section. A variational functional $J\{\Psi_t\}$ is defined in terms of

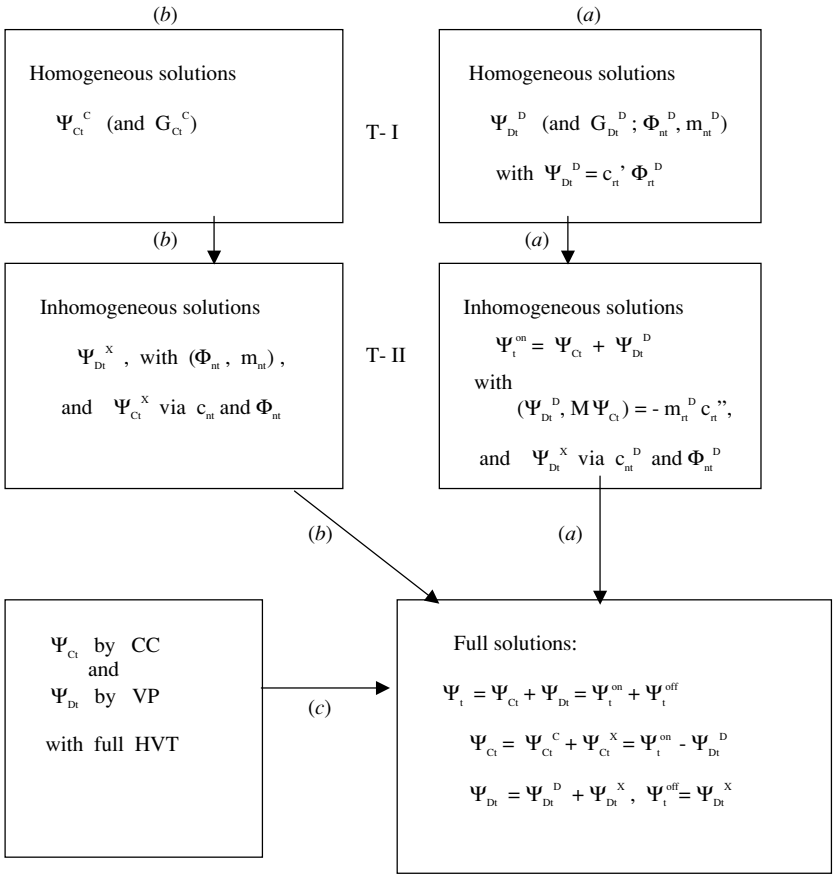

Figure 2. A flow-chart of the two distinct approaches (a) and (b) explored in this paper, where tier 1 (T-1) and tier 2 (T-2) involve different homogeneous and inhomogeneous functions in the D and C components, respectively. Approach (c) is also indicated, explicitly showing the coupled channel (CC) and VP treatments of the two components, and emphasizing the essential dependence on the HVT. All three approaches end up with the total wavefunctions, which, when converged, should be equivalent.

the trial function Ψ_t which may contain one or more linear (c_{st}) and nonlinear (d_q) parameters and approximate amplitudes χ_{it}. That is,

$$J\{\Psi_t\} = \chi_t + (\Psi_t, [H - E]\Psi_t). \tag{2.1a}$$

All the open, as well as closed, channel boundary conditions are assumed to be properly incorporated in the trial function. In general, χ_t is a sum of χ_{ti} with given initial conditions a_i, with $i = 1, \ldots, N_P$, for a total of N_P open channels at a given total energy E. For example, $\chi_{it} = \sum_j a_i K_{ijt} a_j$, for the reactance matrix K. The actual form of the functional can be somewhat different for the Hulthen, Kohn and Schwinger and other types of VP, but our discussion does not depend on its explicit form. The improvements to be made in the next section should be applicable to all cases.

Thus, the trial function in a variational treatment is written conveniently in two parts as

$$\Psi_t = \Psi_{Ct}(\chi_t, a) + \Psi_{Dt}(c, d), \tag{2.1b}$$

where the subscripts C and D simply denote the solutions with emphasis on the asymptotic *channel* and the *dynamic* reaction/diffusion components, respectively. The C part carries exclusively all the open channel boundary conditions in region II, while the D part predominantly describes the reaction zone I, but carries no explicit asymptotic channel information. Besides, the functional form of Ψ_{Ct} is pre-chosen.

These two components overlap (preferably mostly in region III), so that they are *nearly* mutually orthogonal because of spatial separation. In the case of the so-called PQ formulation, as summarized in the appendix, the separation is carried out in some configuration (state) space, to achieve the orthogonal separation. The separation in (2.1) does not require such orthogonalization. The two parts can carry individually much of the overlapping information of region I; obviously this is not economical, and an approximate orthogonalization between the two components may be more effective.

We may set

$$\Psi_{Ct} = \sum_{i=1}^{NC} a_i \Psi_{Cit}(\chi_{it}) \tag{2.1c}$$

for N_C ($\equiv$NC) open channels, where Ψ_{Cit} are further specified as $\Psi_{Cit} = \psi_{it}\ u_{it}$. In the case of a two-cluster channel, for example, the internal cluster function is $\psi_{it} = \psi_{i1t}\psi_{i2t}$, and u_{it} is the inter-cluster function which is expressed in terms of the in-coming and out-going wavefunctions of known forms. (Proper symmetrization is assumed.) By contrast, Ψ_{Dt} describes the scattering function in the diffusion region I, and is usually constructed in terms of square-integrable trial functions Φ_{st} as $\Psi_{Dt} = \sum_{s=1}^{ND} c_{st}\Phi_{st}(d)$, N_D ($\equiv$ND), where c_{st} are the N_D linear variational parameters and the d's are nonlinear parameters, $d\{d_m; m = 1, \ldots, N_d\}$. The conventional VP approach relies on the Ψ_{Dt} part to represent the complicated dynamics in the interaction region, just as in the bound state case, while Ψ_{Ct} covers both regions II and III. The linear parameters in Ψ_{Dt} are then determined by the VP procedure, connecting the two solutions, but the nonlinear parameters d cannot be optimized. Optimal determination of the d's requires criteria outside the VP (section 4). Variations of the functional J with respect to the linear parameters c and amplitudes χ provide the conditions that these parameters must satisfy to make J stationary; that is, the error $\delta\chi_t$ in the calculated χ_t is at least second order in the error $\delta\Psi_t$. Here, the χ_t's behave like linear parameters in so far as the variation of J is concerned. Thus, we have from (2.1) $\delta J/\delta\Psi_t = 0$ which can be rewritten as

$$\delta J/\delta\Psi_{Ct} = 0 \rightarrow \delta J/\delta\chi_{it} = 0, \quad \text{or} \quad \delta J/\delta u_{it} = 0, \quad i = 1, \ldots, N_C, \tag{2.2a}$$

$$\delta J/\delta\Psi_{Dt} = 0 \rightarrow \delta J/\delta c_{st} = 0, \quad s = 1, \ldots, N_D. \tag{2.2b}$$

Equations (2.2) provide a set of algebraic equations that define the variational parameters χ's and c's, and must be solved simultaneously, iteratively. The nonlinear parameters d's are pre-chosen rather arbitrarily, and are again *not* determined by the above variations.

The VP for a scattering system, as defined above, is known (Schwartz 1961a, 1961b) to give wildly fluctuating amplitudes (e.g. tangent of phase shift) for some values of the nonlinear parameters, while forming one or more stable plateau regions for other parameter values, as illustrated in figure 3(*a*). The regions of such unstable fluctuations are *not* sharply defined when the number of linear parameters is small, but become more numerous and exhibit sharper peaks/valleys as more linear parameters are added. The stable plateau regions also become flatter in between the sharp peaks, and eventually the plateaus flatten out, presumably at the 'correct' value for the amplitude. Such erratic behaviour, the difficulty (i), as well as (ii) the lack of criteria for optimization of the solution, was the main reason for retarding the

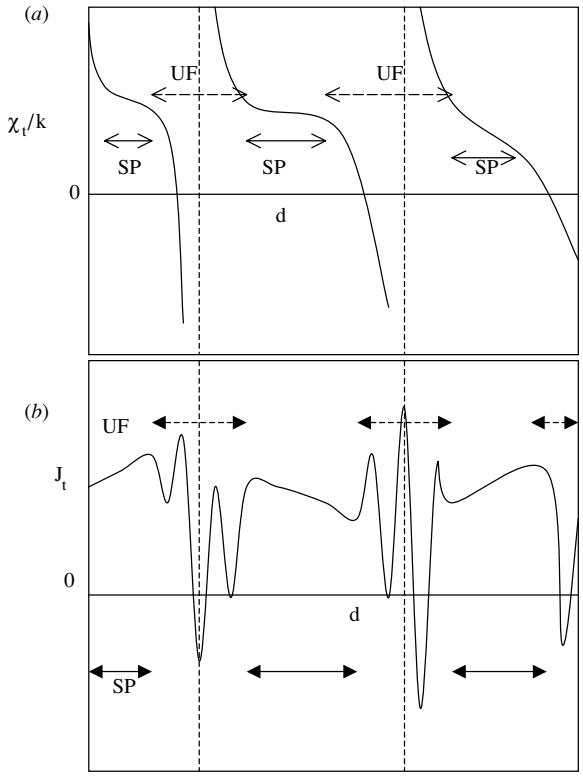

Figure 3. Typical behaviour of a variationally calculated amplitude χ_t as a function of one of the nonlinear parameters d is illustrated, in which both the unstable fluctuating (UF) and stable plateau (SP) regions are indicated. As the number of linear parameters grows, the boundaries between the UF and SP regions become sharper, and presumably the SP regions tend to become more flat around the value of the true amplitude. The calculated amplitude then becomes insensitive to particular values of the nonlinear parameter. $J_t = -iF_t$.

application of VP to scattering systems for all these years. In view of the potentiality of the VP approach in treating region I, we re-examine and improve the method in this paper.

The fluctuations noted above and illustrated in figure 3 are presumably caused by the vanishing denominators of the variationally defined linear parameters, as a direct consequence of the absence of bound property of the operator $M = H - E$. They occur at particular values of nonlinear parameters contained in $\Psi_{\mathrm{D}t}$. First, we analyse the contents of (2.1*b*). Variation of J with respect to the c's gives a set of N_{D} equations for the c's, as

$$c_{st} = -\sum_{s} (\mathbf{M})^{-1}_{su} B_u, \tag{2.3}$$

where $\mathbf{M}$ is an ND $\times$ ND matrix with elements

$$M_{sn} = (\Phi_{st}, M\Phi_{nt}) \qquad \text{and} \qquad B_{nt} = (\Phi_{nt}, M\Psi_{\mathrm{C}t}). \tag{2.4}$$

The inverse of $\mathbf{M}$ involves its determinant, $\det(\mathbf{M}) = \Pi_s m_{st}$, where m_{st} are the roots of $\mathbf{M}$ and the Φ^{D}_{st} are the corresponding orthonormal basis functions. The superscript D denotes the homogeneous solutions, properly orthonormalized. We then have simply

$$c_{st} = -\left(\Phi^{\mathrm{D}}_{st}, M\Psi_{\mathrm{C}t}\right)\big/ m_{st}. \tag{2.5}$$

The roots m_{st} depend on the values of the nonlinear parameters d in the trial functions Φ_{nt}^{D}, which are the linear combinations of Φ_{nt}'s. The fluctuating instability occurs mainly when one or more of these roots m_{st} are close to zero, making the corresponding c_s's very large, to be discussed fully in section 3.

The second source of the difficulty (i) may also be present with $\Psi_{\mathrm{C}t}$ when it is also treated variationally in the original VP. However, as indicated by (2.1c), the form of the $\Psi_{\mathrm{C}t}$ is such that the variations of J with respect to the u's give a set of coupled equations, which can readily be solved exactly, as long as the number of open channels explicitly retained is small. Therefore, throughout the paper, we treat only the complex D part variationally, while the C part is to be solved exactly by the coupled channel method. This is a minor, but practically important, updating of the original VP. This not only makes the present formulation converge to the minimum principle when all the open channels are explicitly included in the C part, but also clearly shows the crucial extension of the theory where the extremum principle becomes inapplicable.

Several attempts have been made in the past (Harris 1967, Nesbet 1969, Callaway 1978, Nesbet 1980) to remedy the difficulty (i), but some of them are either incorrect or not very effective. We present in section 3 a complete discussion of the remedies in a general and coherent picture. It is now apparent from the structure of the coefficients c in (2.5) that the necessary improvement may be carried out in three different, but somewhat related, ways, as the parameter c_r with $m_{rt} \approx 0$ is given in terms of m_{rt}, Φ_{rt}^{D} and $\Psi_{\mathrm{C}t}$. Thus, as illustrated in figure 2, we can proceed in three different but related ways:

(a) Avoid the use of (2.5) for the Φ_{rt}^{D} with $m_{rt} = 0$, and include it in $\Psi_{\mathrm{C}t}$ such that B_{rt} also vanishes.
(b) Definition of m_{rt}^{D} may be changed by using a modified M, similar to M^{DCD} of the appendix, so that the denominator in c_{rt} need not vanish simply because $m_{rt} = 0$.
(c) Finally, Φ_{rt}^{D} may be changed by adjusting the nonlinear parameters, so that none of the m's vanish, and the c's are changed.

Approaches (a) and (b) will be discussed in the next section, the former having been discussed recently (Hahn 2006). The approach (c) is direct and simple, but requires information on the degree of instability and optimization, and thus depends heavily on the hypervirial theorems of section 4.

3. The two-tier approach to improved VP for scattering states

Improvement of the conventional VP to remedy the instability problem discussed in section 2 is very much facilitated by a reformulation of the VP via a two-tier approach. The past conceptual misgiving seems to have been in the combined treatment of the scattering problem using the single functional J, although the trial function is always constructed in two parts as in (2.1) and (2.2). As stressed earlier, it is essential to recognize that the scattering case, with continuous spectrum and non-square integrable wavefunctions (in a Banach space), is mathematically different from the bound state case with discrete point spectrum and square-integrable wavefunctions (in a Hilbert space). The oscillating asymptotic boundary conditions for the open channels require special treatment. Thus, in a typical R-matrix picture (Lane and Thomas 1958, Newton 1982, Goldberger and Watson 1964), the 'interior' interaction region I and the other asymptotic channel region II of figure 1(a) are first treated separately and then joined at region III. By contrast, in the PQ formulation of the appendix, an orthogonal separation is introduced not in the coordinate space, but in the configuration space. Still

another possible approach is to separate the homogeneous and inhomogeneous solutions of the coupled C+D problem, and this aspect is explored below.

The two-tier approach to scattering problems is not new (Hahn 1974a, 1974b), but we emphasize here by explicitly arranging the theory in two tiers, bringing out clearly the homogeneous and inhomogeneous solutions of the fully coupled problem. It would facilitate the removal of the instability difficulty. Thus, tier 1 deals with the homogeneous solutions, both for the C and D components, denoted by the $\Psi_{\rm C}^{\rm C}$ associated with the $\Psi_{\rm C}$ equation (as well as $G_{\rm C}^{\rm C}$) and $\Psi_{\rm D}^{\rm D}$ for $\Psi_{\rm D}$ (and the Green's function $G_{\rm D}^{\rm D}$). The subscript t denotes approximate trial quantities. In tier 2, the coupling between the C and D components is treated; matching the two components in region III is through the determination of the parameters c_n's and χ's in $\Psi_{\rm D}$ and $\Psi_{\rm C}$, respectively. The necessary improvement of the VP to make the solution stable then follows naturally.

The two-tier approach is distinct from the conventional reaction theory with the P–Q operators in that the strong orthogonality requirement $PQ = 0$ is relaxed, although the overall structure is similar. For ready comparison, therefore, the latter is briefly summarized in the appendix. The difficulty of explicitly deriving the operators P and Q is well known and this has no direct relevance to what we discuss below.

Two sets of coupled equations are generated by (2.2), which admit both the homogeneous and inhomogeneous solutions as

$$\Psi_{{\rm C}t} = \Psi_{{\rm C}t}^{\rm C} + \Psi_{{\rm C}t}^{\rm X} \qquad \text{and} \qquad \Psi_{{\rm D}t} = \Psi_{{\rm D}t}^{\rm D} + \Psi_{{\rm D}t}^{\rm X}, \tag{3.1}$$

where the superscripts C and D denote the homogeneous solutions and the X for the inhomogeneous solutions that mix the C and D components. In general, the C and D components are *not mutually orthogonal*, but the usual relations associated with the homogeneous and inhomogeneous solutions exist.

Tier 1. The homogeneous parts of the C and D components are first treated. Thus, we have

$$J_{\rm CC}\{\Psi_{{\rm C}t}^{\rm C}\} = \chi_{{\rm C}t}^{\rm C} + (\Psi_{{\rm C}t}^{\rm C}, M\,\Psi_{{\rm C}t}^{\rm C}) \tag{3.2a}$$

$$J_{\rm DD}\{\Psi_{{\rm D}t}^{\rm D}\} = (\Psi_{{\rm D}t}^{\rm D}, M\Psi_{{\rm D}t}^{\rm D}). \tag{3.2b}$$

Equation (3.2*b*) results in a set of square integrable trial functions and diagonalization of the energy matrix, as in (2.4), resulting in an orthonormal set $\{\Phi_{{\rm D}nt}\}$ and m_{nt}, $n = 1, \ldots, N_{\rm D}$. In particular, for the root $m_{nt} = 0$ (and perhaps for $m_{nt} \approx 0$) (2.5) blows up, and so we set instead

$$\Psi_{{\rm D}t}^{\rm D} = c'_{rt}\,\Phi_{{\rm D}rt} \qquad \text{with} \qquad m_{rt} = 0, \tag{3.3}$$

where c'_{rt} is yet unspecified. This is the 'on-shell' part of $\Psi_{{\rm D}t}$, and in principle could be included in the channel part $\Psi_{{\rm C}t}$ which represents mainly the on-shell part of the solution. In fact, this was done in resolving the difficulty (i) in the approach (a), as proposed recently (Hahn 2006). With the $\Psi_{{\rm D}t}^{\rm D}$ included in $\Psi_{{\rm C}t}$, the two rearranged functions

$$\Psi_t^{\rm on} = \Psi_{{\rm C}t} + \Psi_{{\rm D}t}^{\rm D} \qquad \text{and} \qquad \Psi_t^{\rm off} = \Psi_{{\rm D}t} - \Psi_{{\rm D}t}^{\rm D} \tag{3.1a}$$

are now roughly orthogonal to each other (provided $\Psi_t^{\rm on} \propto \Psi_{{\rm D}t}^{\rm D}$ in region I). In so far as the C part is concerned, we assume that the exact numerical solutions $\Psi_{{\rm C}t}^{\rm C}$ of the homogeneous equations derived by (2.2) can be obtained, rather than treating it variationally.

Tier 2. Calculation of the inhomogeneous solutions involves the Green functions for the homogeneous equations. The necessary functionals that employ the homogeneous solutions

obtained above can then be written, following the structure of the equations similar to (A.4), as

$$J_{\mathrm{C}}\{\Psi_{\mathrm{C}t}\} = \chi_t + \big(\Psi_{\mathrm{C}t}, \big[M + MG^{\mathrm{D}}_{\mathrm{D}t}M\big]\Psi_{\mathrm{C}t}\big) + 2\big(\Psi_{\mathrm{C}t}, M\Psi^{\mathrm{D}}_{\mathrm{D}t}\big) \tag{3.4a}$$

$$J_{\mathrm{D}}\{\Psi_{\mathrm{D}t}\} = \big(\Psi_{\mathrm{D}t}, \big[M + MG^{\mathrm{C}}_{\mathrm{C}t}M\big]\Psi_{\mathrm{D}t}\big) + 2\big(\Psi_{\mathrm{D}t}, M\Psi^{\mathrm{C}}_{\mathrm{C}t}\big). \tag{3.4b}$$

It is noted that (3.4*a*) and (3.4*b*) are mathematically disjoint, as for example $\Psi_{\mathrm{C}t}$ in (3.4*a*) is determined without the $\Psi_{\mathrm{D}t}$, or rather $\Psi^{\mathrm{X}}_{\mathrm{D}t}$, and vice versa for the $\Psi_{\mathrm{D}t}$ without the $\Psi^{\mathrm{X}}_{\mathrm{C}t}$ in (3.4*b*).

First for the D part. Within the space spanned by the set generated in (2.4), we may write the Green function and the inhomogeneous solutions as

$$G^{\mathrm{D}}_{\mathrm{D}t} = \sum_{n\neq r}^{\mathrm{ND}} (\Phi_{\mathrm{D}nt})\, m^{-1}_{nt} (\Phi_{\mathrm{D}nt}) \tag{3.5}$$

and

$$\Psi^{X}_{\mathrm{D}t} = \sum_{n\neq r}{}' c_{nt}\Phi_{\mathrm{D}nt}, \tag{3.6}$$

where c_{nt} are to be determined by the matching, as in (2.5), and the sum does not include the $m_{rt} = 0$. On the other hand, the inhomogeneous solution $\Psi^{\mathrm{X}}_{\mathrm{C}t}$ of the C part requires an explicit evaluation of the $G^{\mathrm{C}}_{\mathrm{C}t}$ associated with the homogeneous equations. Such functions are often difficult to evaluate, but, since $G^{\mathrm{C}}_{\mathrm{C}t}$ exclusively appears in $\Psi^{\mathrm{X}}_{\mathrm{C}t}$ only, its effect can be dealt with by directly solving the relevant coupled equations for Ψ^{on}_t, with proper outgoing (or the cosine functions) boundary conditions, and the relevant part $\Psi^{\mathrm{X}}_{\mathrm{C}t}$ can be separated from $\Psi_{\mathrm{C}t}$. The $MG^{\mathrm{C}}_{\mathrm{C}t}M$ term in (3.4*b*) provides the necessary shift, and decouples the two components. Thus, variations of J_{D} give immediately a ND × ND energy matrix of $M^{\mathrm{C}} = M + MG^{\mathrm{C}}_{\mathrm{C}t}M$ to be diagonalized. The new set $\Phi^{\mathrm{C}}_{\mathrm{D}nt}$ and m^{C}_{nt} are such that $m^{\mathrm{C}}_{nt} \approx m_{nt} + \Delta_{nt}$, where n includes the state r for which we had originally $m_{rt} = 0$. We now have

$$c^{\mathrm{C}}_{nt} = -B^{\mathrm{C}}_{nt}/m^{\mathrm{C}}_{nt}, \qquad \text{where} \quad B^{\mathrm{C}}_{nt} = \big(\Phi^{\mathrm{C}}_{nt}, M\Psi_{\mathrm{C}t}\big), \tag{3.7}$$

for all n, including $n = r$. Thus, we no longer have any of the c^{C}_{nt} blowing up. This is the approach (b) via the two-tier formulation and the instability difficulty (i) has been resolved. Of course, when the C component contains all the strongly coupled channels, we expect (Hahn 1970) a strong $G^{\mathrm{C}}_{\mathrm{C}t}$ such that Δ_{nt} is large for all n (and perhaps even $m^{\mathrm{C}}_{nt} > 0$).

To focus specifically on the inhomogeneous solutions, we may replace (3.4) by a simpler set of functionals which do not contain the approximate Green functions, specifically the $\mathrm{G}^{\mathrm{C}}_{\mathrm{C}t}$. We have

$$J'_{\mathrm{C}}\big\{\Psi^{X}_{\mathrm{C}t}\big\} = \chi^{\mathrm{D}} + \big(\Psi^{X}_{\mathrm{C}t}, M\Psi^{X}_{\mathrm{C}t}\big) + 2\big(\Psi^{X}_{\mathrm{C}t}, M\Phi_{\mathrm{D}rt}\big)c'_{rt} + 2\big(\Psi^{X}_{\mathrm{C}t}, M\Psi^{X}_{\mathrm{D}t}\big) \tag{3.8a}$$

$$J'_{\mathrm{D}}\big\{\Psi^{X}_{\mathrm{D}t}\big\} = \big(\Psi^{X}_{\mathrm{D}t}, M\Psi^{X}_{\mathrm{D}t}\big) + 2\big(\Psi^{X}_{\mathrm{D}t}, M\Psi^{\mathrm{C}}_{\mathrm{C}t}\big) + 2\big(\Psi^{X}_{\mathrm{D}t}, M\Psi^{X}_{\mathrm{C}t}\big). \tag{3.8b}$$

The variation $\delta J'_{\mathrm{D}}/\delta\Psi^{X}_{\mathrm{D}t} = 0$ gives $c_{nt} = -B_{\mathrm{D}nt}/m_{nt}$, $n \neq r$, where $B_{\mathrm{D}nt} = (\Phi_{nt}, M\Psi_{\mathrm{C}t})$. However, since $B_{\mathrm{D}nt}$ contain two terms, $B_{\mathrm{D}nt} = B^{\mathrm{C}}_{\mathrm{D}nt} + c_{nt}\Delta_{nt}$, we have $c_{nt} = -B^{\mathrm{C}}_{\mathrm{D}nt}/[m_{nt} + \Delta_{nt}]$, where $B^{\mathrm{C}}_{\mathrm{D}nt} = \big(\Phi_{\mathrm{D}nt}, M\Psi^{\mathrm{C}}_{\mathrm{C}t}\big)$, as in (3.7), and $\Delta_{nt} = \big(\Phi_{\mathrm{D}nt}, MG^{\mathrm{C}}_{\mathrm{C}t}M\Phi_{\mathrm{D}nt}\big)$. That is, $c_{nt} \approx c^{\mathrm{C}}_{nt}$ of (3.7). Generally, the shifts Δ_{nt} are large when the m's represent pseudostates, while they become rather small for true resonances due probably to the orthogonality relations discussed in the appendix.

We have described above the approach (b) in a mathematically transparent way, and now consider the equivalence between the approach (b) described above and that of (a) proposed recently (Hahn 2006), both designed for removing the difficulty (i). In fact, in (3.3), we noted that the parameter c'_{rt} in $\Psi^{\mathrm{D}}_{\mathrm{D}t}$ was not yet defined. It appears on the inhomogeneous term in J_{C} and thus $\Psi^{\mathrm{X}}_{\mathrm{C}t}$ will depend on it. As a consistency condition, we then required in approach (a) that the integral

$$(\Phi_{rt}, M\Psi_{\mathrm{C}t}) = -m_{rt}c''_{rt} \qquad (=0 \quad \text{for} \quad m_{rt} = 0) \tag{3.9}$$

give $c''_{rt} = c'_{rt}$. (3.9) implies that the right-hand side can vanish because of m_{rt}, but not by c''_{rt}.

To further show the equivalence between the results obtained by (3.8) and (3.9), we assume that $\Psi_{\mathrm{D}t}(c^a_{rt}) = \Psi^{\mathrm{X}}_{\mathrm{D}t} + c^a_{rt}\Phi_{\mathrm{D}rt}$ and construct a functional

$$J''_{\mathrm{D}}\{\Psi^{X}_{\mathrm{D}t}, c^a_{rt}, c^b_{rt}\} = \big(\Psi_{\mathrm{D}t}(c^a_{rt}), M\Psi_{\mathrm{D}t}(c^a_{rt})\big) + 2\big(\Psi_{\mathrm{D}t}(c^a_{rt}), M\Psi^{\mathrm{C}}_{\mathrm{C}t}\big) + 2\big(\Psi_{\mathrm{D}t}(c^a_{rt}), M\Psi^{X}_{\mathrm{C}t}(c^b_{rt})\big), \tag{3.10}$$

where the c_{rt} dependence is explicitly exhibited, distinguishing the two, c^a_{rt} associated with $\Psi_{\mathrm{D}t}$ and the other c^b_{rt} with $\Psi^{\mathrm{X}}_{\mathrm{C}t}$. Now, if c^b_{rt} in the last term of (3.10) is held fixed during the variation of c^a_{rt}, we are back to (2.1) and (2.2), and the difficulty (i) remains. On the other hand, if we let $c^a_{rt} = c^b_{rt}$ and let them vary together, we have essentially recovered (3.8*b*), without the explicit use of the Green function. This is the contents of the consistency condition (3.9) for the normalization c_{rt} of $\Psi^{\mathrm{D}}_{\mathrm{D}rt}$. Of course, in original (3.8*b*), the functional does not include this homogeneous term, so that no difficulty (i) appears. This concludes the equivalence proof.

The approach (a) was formulated in a somewhat intuitive way, mainly to simplify the calculational procedure. But its theoretical basis is presented here, showing that the remedy for the difficulty one is uniquely given by either (a) or (b). Furthermore, still simpler approach (c) will be discussed in section 4, as it depends heavily on the hypervirial theorems. In some previous treatments of the difficulty (i), the c_{rt} that controls the short-range behaviour was mixed up with the amplitude χ_t that is prominent only in the asymptotic region. It should also be noted that, as the homogeneous parts ($\Psi^{\mathrm{C}}_{\mathrm{C}t}$ and $G^{\mathrm{C}}_{\mathrm{C}t}$) of the C sector improve, with more open channels added, the theory based on (3.4) approaches the minimum principle, mainly because of the orthogonality relations (A.5) of the appendix.

4. Quality test of approximate solutions and the hypervirial theorems

We now discuss the shortcoming (ii) of the conventional VP, that is, lack of criteria to judge the 'goodness' of a solution, and also to optimize the nonlinear parameters in the variationally determined solution. Although the improved VP formulated in section 3 should eventually converge to the correct solution, not necessarily monotonically, the availability of a criterion to test the quality of the solution and optimizing it will make the VP more readily applicable. In this section, we consider the hypervirial theorems (HVT) that may provide such a constraint.

The HVT were studied previously (Hirschfelder 1960, Epstein and Hirschfelder 1961, Epstein and Robinson 1963, Demkov 1961, McElroy and Hirshfelder 1963, Robinson and Hirschfelder 1963), mainly to derive relationships between the wavefunctions and phase shifts. Some perturbative HVT approaches were also studied (Killingbeck *et al* 2001, 2004). Presumably, previous applications of the HVT to scattering states have been limited because of the presence of the instability problem (i); the HVT is inoperative when the nonlinear parameters are in one of the unstable zones. Therefore, the formulation of section 3 that places the solution in the stable region is crucial in making the HVT effective. In fact, the hypervirial integrals are very sensitive to the amplitude fluctuations, and this sensitivity can in turn be used with great advantage to identify the unstable regions.

(4.a) The HVT is derived from the identities $(\Psi'', WM\Psi') = 0$ and $(M\Psi', W\Psi'') = 0$, where Ψ' and Ψ'' are the two degenerate exact scattering solutions and where W is a so far arbitrary virial operator, and we have $M = H - E$, $H = K + V$. By partial integrations of the second integral, and then subtracting the first integral from it, we have the general virial integral

$$R = F + \{BC; K) = 0 \tag{4.1a}$$

with

$$F \equiv (\Psi'', [M, W]\Psi') = (\Psi'', [H, W]\Psi'), \tag{4.1b}$$

where $\{BC; K\}$ denotes the boundary contribution coming from the partial integrations that involve the kinetic energy operator K. That is, in a one-particle system, for example,

$$\{BC; K\} = -(1/2) \int [(W\Psi'')\nabla\Psi' - \Psi'\nabla(W\Psi'')]\, \mathrm{d}S. \tag{4.2}$$

Note that the expression for F is explicitly E independent; only the wavefunctions carry this information when M is replaced by H in the commutator. The two expressions are of course completely equivalent. With $\Psi' = \Psi''$ and choosing a special W such that $\{BC\} = 0$, we have $R = F$.

When the exact Ψ's in F are replaced by an approximate solution Ψ_a (subscript a to distinguish from the variational functions with the subscript t), we have the corresponding F_a given by

$$F_a = (\Psi_a, [M, W]\Psi_a) \equiv (\Psi_a, [H, W]\Psi_a), \tag{4.3}$$

where the integration volume need not be the full coordinate space. Although the error function $\varphi_a \equiv \Psi_a - \Psi$ is not known in general, the quantity $M\Psi_a = \xi_a$ can be calculated explicitly, and this is the theoretical basis of F_a as a test integral. The two expressions in (4.3) are equivalent, but the first integral involving $M = H - E$ illustrates the error content of F_a more explicitly (Hahn and Zerrad 2006a, 2006b). Thus, as the Ψ_a improves and approaches the exact solution, we expect the F_a to vanish

$$F_a]_{SP} \to F = 0 \quad \text{as} \quad \Psi_a \to \Psi, \tag{4.4}$$

provided that the approximate solution is in the stable plateau (SP) zone.

The virial operator W is so far unspecified, except for the boundary behaviour. There are many possible choices; following the original virial theorem, we may construct for example a form $W = f \bullet \sum_{i=1}^{N} r_i \bullet p_i$, where f decays to zero at the boundaries, not necessarily at $r_i \to \bullet$. Typical forms for f may be $r^m \exp(-\alpha r)$ or $r^m \exp[-\beta(r - a_n)^2]$, with $m = 0, 1, 2, \ldots$, etc.

Several comments are in order. First, the virial integral (4.1) is satisfied if the Ψ's are the solutions of the scattering equation, independent of the size of the integration volumes involved, because $M\Psi = 0$ is valid locally. Therefore, (4.3) may be used to test the approximate solutions locally in a small volume, or over the full configuration space. Secondly, because of the presence of the commutator, (4.4) is a necessary but not a sufficient condition for the correct solution. That is, for some simple choices of W or Ψ_a, F_a may vanish identically. This spurious cancellation of the integrand and thus F_a itself is the *basic weakness* of the HVT as a test. A partial remedy is to introduce an anti-commutator $F_a^{(+)} = (\Psi_a, \{M, W\}_+\Psi_a)$, which should also vanish for the exact solution and is now explicitly E dependent. Thirdly, by a proper choice of W, we made the BC terms vanish in (4.3). The resulting HVT can thus be applied simply to scattering problems, as with the usual virial theorem for the bound states. Evidently, such a form of HVT cannot test the boundary conditions.

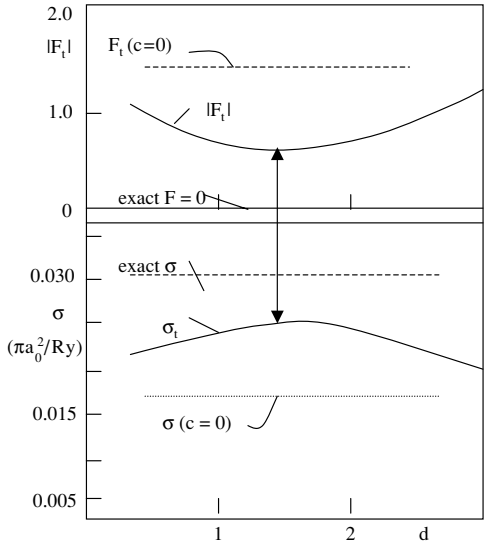

Figure 4. Typical behaviour of the virial integral and correlation between the virial integral F and the calculated cross section is displayed as functions of one of the nonlinear parameters in Ψ_{Qt}. The example chosen is the collisional ionization cross section, evaluated by the generalized Hartree–Fock approach and configuration mixing with one linear parameter c. The quasi-extremum feature between $|F_a|$ and the energy differential cross section σ_a has been attained by a careful construction of the trial functions in the improved VP and the use of a HVT. Of course, such a correlation is possible if and only if all the nonlinear parameters are in one of the stable plateau regions of parameter space. Application of the theory to an actual realistic ionization model bears this out. Although $|F_t|$ is expected to become smaller as the trial function improves, the calculated cross section may assume a maximum, as illustrated here, or a minimum (in an inverted form), depending on the magnitude of the phase shifts (or K matrix), in different quadrants.

As the nonlinear parameters d's in Ψ_{Dt} for example are varied, but still remaining within the stable region, it is possible to find the 'bottom' of the stable hyperplane in the parameter space by watching the magnitude of the $|F_a|$ integrals; the bottom of the plane is indicated by the minimum of $|F_a|$, as illustrated in figures 4 and 5. The smallest $|F_a|$ corresponds to the 'best' choice of the variational parameters. A similar feature was found in an extensive numerical study of some model systems (Hahn and Zerrad 2006a, 2006b). With all the nonlinear parameters in the plateau regions, we then have a pseudo-minimum principle in the form

$$\text{Min}|F_a|]_{\text{SP}} \quad \Rightarrow \quad [\text{the best set of variational parameters}], \tag{4.5}$$

where, unlike in the previous minimum principles, the boundedness of the energy operator M and its modified forms are *not* required. However, two cautionary points must be noted; the convergence discussed above may not always be monotonic, and sometimes breaks down, possibly due to *spurious* cancellations in the virial integrals. Further, for a localized W, for example, an improvement in the wavefunction in one limited area may not necessarily give an improved scattering solution. To avoid this problem, more than one area in the configuration space may be tested.

(4.b) HVT and variational wavefunctions. Form (4.3) is not yet in a useful form to rectify the shortcoming (ii). For both bound and scattering states, consider the single HVT integral

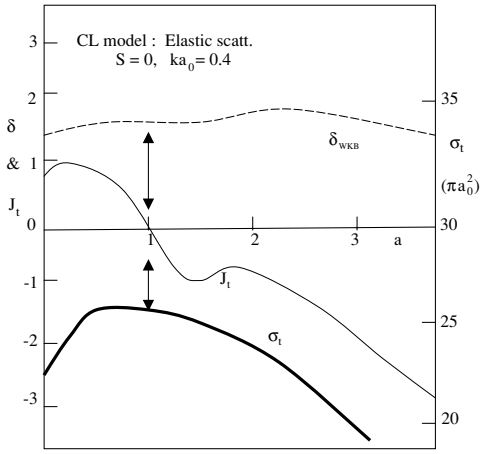

Figure 5. Sensitivity of the virial integrals $J_t = -iF_t$ to unstable fluctuations of variational wavefunctions is illustrated, and is compared with that of the amplitudes, all as functions of nonlinear parameter sets in a N_d dimensional hyperspace, denoted simply by d. This property may be used to sharply define the unstable fluctuating (UF) and stable plateau (SP) regions of the nonlinear parameter space. (See figure 3) Since the HVT is effective only for those functions with the parameters in the SP regions, identification of the SP region becomes important in validating the behaviour (4.3) and (4.4). The solid line arrows indicate the SP zones, while the dashed arrows show the UF regions. Usually, the 'best' nonlinear parameter set occurs near the SP/UF boundaries, as expected from the discussion given in section 3.

in a slightly different form as

$$\begin{aligned} R_t &= (\Psi_t, W[E-H]\Psi_t) = (\Psi_t, W[E-H]\varphi_t) \\ &= (H\Psi_t, W\varphi_t) - (\Psi_t, WH\varphi_t) \\ &= (\Psi_t, [H, W]\varphi_t) + \{BC; K, \varphi_t\}, \end{aligned} \tag{4.6a}$$

which explicitly shows the first-order error term in terms of the error function $\varphi_t = \Psi_t - \Psi$, for the trial and exact wavefunctions, Ψ_t and Ψ, respectively. Again we have $M\Psi = 0$ and $M\Psi_t = M\varphi_t$. Equation (4.6*a*) explicitly shows that the hypervirial integral examines the error in the approximate solution. As $\Psi_t \to \Psi$, we expect $R_t \to 0$.

Furthermore, for W which does not necessarily vanish at the boundaries, R_t is related to $F_t = (\Psi_t, [H, W]\ \Psi_t) = (\Psi_t, [M, W]\Psi_t)$ by

$$R_t = F_t - (M\Psi_a, W\Psi_a) + \{BC; K|\Psi_a, W\Psi_a\}. \tag{4.6b}$$

The difference between the R_a and F_a in (4.6*b*) goes to zero with improved functions and for vanishing boundary contributions, but for approximate solutions, this difference may be significant and useful in applications.

We show below that any variationally determined solutions automatically satisfy the HVT, for all W, to first order in the error function φ_t. For a variational principle, with the trial function $\Psi_a \to \Psi_t$, we have the usual VP given by

$$\delta\chi \approx (\Psi_t, [E-H]\Psi_t), \qquad \text{with} \quad (\Psi_t, [E-H]\varphi_t) \approx 0, \tag{4.7}$$

to second order in $\varphi_t \equiv \Psi_t - \Psi$. Here the variationally determined E_t is replaced by its exact value, as the error is also of second order. That is, the first-order terms in the variational integrals are made to vanish. Note that, with $W = 1$, (4.5) becomes a variational integral of section 2.

Now, we compare (4.5) and (4.6). Since the virial operator W is still left unspecified, we may set the error function φ_t to be of the form [15]

$$\varphi_t = \mathrm{i}W\Psi_t. \tag{4.8}$$

Substitution of (4.8) into the variational integrals in (4.6) gives

$$0 \approx (\Psi_t, [E-H]W\Psi_t) \approx (H\Psi_t, W\Psi_t) - (\Psi_t, HW\Psi_t) = (\Psi_t, [H, W]\Psi_t) - \{BC\}_t, \tag{4.9}$$

which is precisely (4.5), all valid to second order in φ_t. That is, all the terms in (4.5) and (4.6), which are linear in φ_t, drop out. Therefore, in so far as the variationally determined wavefunctions are concerned, the HVT integrals with the variational Ψ_t vanish to first order for all W, and thus provide no additional information on the quality of the solutions. This equivalence proof between the VP and HVT depends on the special choice (4.8) as well as on W, and does not imply that one can replace the VP by HVT or vice versa.

Now, with the HVT available, we can consider the third option (c) of fixing the VP, as mentioned in section 3. That is, the nonlinear parameters in $\Psi_{\mathrm{D}a}$ may be varied in such a way that any zero roots m_{rt} may disappear. However, this can be carried out sensibly only if the variation places the parameters in the stable zone. As noted earlier, the use of the HVT is thus essential in facilitating this procedure, not only in searching the stable zone in the parameter space, but also to optimize the solution. The final solution must be the same as that produced by approaches (a) and (b) discussed in section 3. Because the search for the SP region using the HVT is equivalent to the procedures of (a) and (b), the optimization is carried out in all three cases using the HVT. Obviously, approach (c) relies entirely on the HVT. Usually, it has been found that the 'best' set of nonlinear parameters is given close to the edge of the stable zone.

The HVT is especially effective when only a few linear parameters are involved. Unlike in the conventional VP treatment of the scattering problems, where a large number of linear parameters are usually required before the solution starts to settle, we can obtain with this improved VP/HVT approach a sensible amplitude even when only a few linear parameters are involved.

5. Summary and discussion

We have reformulated the multichannel scattering theory as a two-tier approach, in which both the instability difficulty (i) and the lack of test criteria (ii) are treated in a natural and mathematically consistent way. A set of strongly coupled channels is explicitly described in the channel component $\Psi_{\mathrm{C}t}$, while many (often infinite in number) weakly coupled channels may be omitted for practical reasons. This omission in turn takes away the bound property of the theory and introduces the difficulty (i). Three different, but mathematically equivalent, approaches have been discussed for (i). Thus, the troublesome component in the $\Psi_{\mathrm{D}t}$ is identified and properly treated, either incorporating it in the modified Hamiltonian, as in (3.4) and (3.8) or shifting it to the channel part $\Psi_{\mathrm{C}t}$, as in (3.1a) and (3.9). The coefficient c_{rt} associated with the root $m_{rt} = 0$ is, instead of blowing-up, determined in terms of the shift and/or by the new consistency condition. The very component that gives rise to the breakdown of the VP and instability has been retained. The theory is now stable, without the difficulty (i).

For optimization of nonlinear parameters, the shortcoming (ii) of the conventional VP is rectified by introducing the HVT in section 4, which is effective only if the nonlinear parameters are already in one of the stable regions of the parameter space. The virial integral $F_a = (\Psi_a, [W, H]\Psi_a)$ is made simple by a suitable choice of W, which resembles the theorems

for the bound states. Thus we have Min $|F_a|$ for a optimal set of nonlinear parameters. Several possible choices for W have been discussed, including that decay asymptotically to erase the boundary contribution. This aspect of the problem will be discussed further with numerical examples in a separate report (Hahn and Zerrad 2006a, 2006b), where the applicability of the HVT with various practical constraints is examined. Several applications of the theory to specific scattering (and breakup) systems are in progress, the detailed results of which will be reported elsewhere (Zerrad and Hahn 2006).

The main result of this paper is given by (3.4)/(3.8), (3.9)/(3.1a) and (4.3)/(4.4). The improved VP with HVT is now applicable to scattering systems, *almost* as effective as the Ritz principle is for the bound states and the minimum principles for low energy scattering, even when parts of weakly coupled open channels are omitted and the bound property is absent. The HVT have to be used with caution, however, since the $|F_a| = 0$ is not a sufficient condition for the improved solution. With more of the strongly coupled channels retained, we expect that the theory should become more robust and *effective*, while the previous approaches with the bound property *break down*. Of course when all the open channels are explicitly included in Ψ_{Ca}, the present theory converges to that of the minimum principle. The theory of sections 3 and 4 is a direct extension to higher energies of the usual coupled channel method with pseudo-potentials (-states), where the ever-present problems of (i) and (ii) have been resolved. The HVT plays an essential role in optimizing the potential parameters.

The unitarity correction for the neglected, and presumably weakly coupled, open channels becomes important, especially when some of the neglected channels are collectively also strongly coupled. A number of known methods can be applied, including the all-inclusive projection operators in the semiclassical approximation (Hahn and Watson 1972, 1973), but this problem warrants a careful discussion elsewhere.

6. Appendix. Formal structure of the reaction theory

This appendix summarizes a typical reaction theory that provides a guide to the overall structure of the two-tier approach given in section 3, but much of the details, including the orthogonality property, are quite different. It is in sharp contrast with the R-matrix formulation.

In terms of a set of projection operators P and Q, with $P + Q = 1$ and $PQ = 0$, the scattering problem is divided into two 'orthogonal' parts, one (P) describing the open channels and the other (Q) for the closed channels. Then, in the usual way, we have, with $M = H - E$,

$$PMP\,\Psi = -PMQ\,\Psi \tag{A.1a}$$

$$QMQ\,\Psi = -QMP\,\Psi. \tag{A.1b}$$

In the *MP* developed previously (Hahn and Spruch 1967), the bound property $QMQ > 0$ was the key feature. The P equations generally admit a homogeneous solution, i.e. $PMP\Psi^P = 0$, so that $P\Psi$ contains two parts, as $P\Psi = P\Psi^P + P\Psi^{PQ}$, where the first part is independent of the Q component, while the second part depends explicitly on $Q\Psi$.

Similarly, the $Q\Psi$ part can also be written as $Q\Psi = Q\Psi^Q + Q\Psi^{QP}$, where $Q\Psi^Q$ is the homogeneous solution, $QMQ\Psi^Q = 0$ and is independent of $P\Psi$, while $Q\Psi^{QP}$ is the inhomogeneous solution of (3.4a) and explicitly dependent on $P\Psi$. In the conventional formulation, where the exact, and mutually orthogonal P and Q are assumed, the $Q\Psi^Q$ is absent, except for possible resonances. Therefore, we include this term in a curly bracket, and write (A.1) as

$$PMP\,\Psi^{PQ} = -PMQ\,\Psi^{QP} - PM\{Q\Psi^Q\} \tag{A.2a}$$

$$QMQ\,\Psi^{QP} = -QMP\Psi^{PQ} - QMP\Psi^{P}, \tag{A.2b}$$

which are quite symmetric in the P and Q components. The two sets are still coupled, through the first term on the right in each equation. For the two homogeneous equations, their normalizations are not trivial. For $P\Psi^P$, the asymptotic boundary condition fixes its normalization uniquely. On the other hand, it is not obvious that the theory can fix the normalization of the $Q\Psi^Q$, and this is related to the difficulty (A), as will be shown below.

To make the formal analysis complete, we go one step further and write the solutions of (A.2) formally as

$$P\Psi = P\Psi^P + G^P M\{Q\Psi^Q\} + G^P MQ\Psi^{QP} \equiv P\Psi^P + P\Psi^{PQ}, \quad \text{with} \quad G^P = -(PMP)^{-1} \tag{A.3a}$$

$$Q\Psi = Q\Psi^Q + G^Q MP\Psi^P + G^Q MP\Psi^{PQ} \equiv \{Q\Psi^Q\} + Q\Psi^{QP}, \quad \text{with} \quad G^Q = -(QMQ)^{-1}. \tag{A.3b}$$

Again, when the term $\{Q\Psi^Q\}$ is included, we have a completely symmetric situation. (A.3) in turn give the uncoupled equations

$$PM^{PQP}P\Psi^{PQ} \approx P(M + MG^Q M)P\Psi^{PQ} = -PM\{Q\Psi^Q\} - PMG^Q MP\Psi^P \tag{A.4a}$$

$$QM^{QPQ}Q\Psi^{QP} \equiv Q(M + MG^P M)\,Q\Psi^{QP} = -QMP\Psi^P - QMG^P M\{Q\Psi^Q\}. \tag{A.4b}$$

These two equations are now uncoupled; the right-hand sides are given purely in terms of the homogeneous solutions, so that they are determined once and for all before the coupling between the P and the Q parts is considered. The set is of course somewhat different from the well-known forms, because of the right-hand sides in (3.4).

An important orthogonality property emerges from the above expressions, i.e. due to the properties of the Green functions, we have (Hahn 1969, 1970)

$$PM^{PQP}P = M^{PQP} \quad \text{and thus} \quad QM^{PQP} = 0 = M^{PQP}Q \tag{A.5a}$$

$$QM^{QPQ}Q = M^{QPQ} \quad \text{and thus} \quad PM^{QPQ} = 0 = M^{QPQ}P, \tag{A.5b}$$

and similarly

$$QMP\Psi^P = MP\Psi^P, \quad \text{since} \quad PMP\Psi^P = 0 \tag{A.6a}$$

$$PMQ\Psi^Q = MQ\Psi^Q, \quad \text{since} \quad QMQ\Psi^Q = 0. \tag{A.6b}$$

Thus, the two operators M^{QPQ} and M^{PQP} are automatically in the Q and P spaces, respectively, even without the projections. This property (A.5), together with (A.6) which are important in normalizing the homogeneous solutions, was used earlier in relaxing the minimum principle by eliminating the projection operators altogether. The orthogonality property (A.6*a*) also justifies the rather clumsy superscripts in the operators.

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