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Variational many-channel nuclear reaction formalism*

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We present multichannel nuclear reaction formalisms based on the Schwinger and Kohn variational principles. Our formalisms seem somewhat simpler in form than those heretofore proposed. The necessity of using the entire set of asymptotic boundary conditions to constrain the trial wave function is stressed. We show how this may be done by employing the coupled integral equations formalism discussed by Baer and Kouri, Kouri and Levin, and by Tobocman. Several explicit expressions for the transition amplitude are presented which appear to provide a promising basis for doing many-body system scattering reaction calculations.

[NUCLEAR REACTIONS Variational multipartition nuclear reaction formalism; coupled LS equation method used to impose all asymptotic boundary condition constraints.]

I. INTRODUCTION

The literature contains several many-body versions of the Lippmann-Schwinger[1] and Kohn[2] variational principles.[3] Of particular interest to us was the employment of the Schwinger variational principle by Hüfner and Lemmer[4] as the basis for using nonperturbative Hilbert space truncation methods (like the shell model or random phase approximation) for the calculation of elastic and inelastic scattering transition amplitudes for nucleon-nucleus collisions. This formalism was found to be superior to several other methods when tested on a simple two-body, two-channel model.[5]

Except for those treatments[6] of the three-body system which base themselves on the Faddeev equations instead of the Lippmann-Schwinger equations, none of these variational principle formalisms deal adequately if at all with the special problem posed by the existence of more than one reaction channel. The problem is how to constrain the trial wave function (or wave matrix operator) to simultaneously fulfill appropriate boundary conditions in all channels.

In this article we present relatively simple multichannel formulations of the Schwinger and Kohn variational principles. The importance of imposing the complete set of asymptotic boundary condition constraints on the trial wave matrix operator is demonstrated. It is shown that the wave matrix operator must be the simultaneous solution of N integral equations, one for each partition (or family of channels associated with a particular mode of separating the particles into two groups). Each of these integral equations contains a distinct asymptotic boundary condition constraint. Each of these integral equations has a kernel which is not completely continuous and so the integral equation is not susceptible to solution by conventional methods.

By means of the methods of Baer and Kouri,[7] of Kouri and Levin,[8] and of Tobocman[9] these integral equations can be coupled together in such a way as to yield an integral equation for the wave matrix which has a completely continuous kernel that incorporates the complete set of asymptotic boundary condition constraints. This result is incorporated into our multichannel variational principle. Several explicit expressions for the transition amplitude are presented which appear to provide a promising basis for doing many-body system scattering reaction calculations.

Our approach is an alternative to the Faddeev approach which has the advantage that the formalism has the same structure for the n-body system as it does for the three-body system.

In Sec. II the Schwinger variational principle is generalized from the single-partition version of Hüfner and Lemmer to a many-partition version. This provides a variational expression for the transition amplitude to be used in conjunction with approximate expressions for the scattering state wave functions or approximate expressions for the transition operator. In Sec. III it is shown how to generate formal solutions of the integral equations for the transition operator which are constrained by the entire set of asymptotic boundary conditions. In Sec. IV the problem of disconnected graphs is addressed. In Sec. V it is shown that the Kohn variational principle may be generalized to include possible rearrangements in the same fashion as the Schwinger variational principle. Useful explicit expressions for the transition amplitude and the variational functions are presented in Sec. VI. The results are summarized in Sec. VII.

II. SCHWINGER VARIATIONAL PRINCIPLE FOR THE MANY-BODY PROBLEM

Consider a system of N distinguishable particles. (If the particles are indistinguishable, then one must make appropriately symmetrized sums of transition amplitudes calculated on the assumption of distinguishability.[10]) For each partition $\alpha, \beta, \ldots$ of the particles into two clusters there is a decomposition of the Hamiltonian into two parts:

$$H = H_\alpha + V_\alpha = H_\beta + V_\beta = \cdots .$$

H_α contains the kinetic energy and the intracluster interactions while V_α is the sum of intercluster interactions for partition α. Let ϕ_a be a continuum eigenstate of H_α and let $\psi_a^{(+)}$ and $\psi_a^{(-)}$ be the associated scattering states.

$$(E - H_\alpha)\phi_a = 0 , \tag{1a}$$

$$\psi_a^{(+)} = \phi_a + G_\alpha V_\alpha \psi_a^{(+)} , \tag{1b}$$

$$\psi_a^{(-)} = \phi_a + G_a^\dagger V_\alpha^\dagger \psi_a^{(-)} , \tag{1c}$$

$$G_\alpha = (E - H_\alpha)^{-1} . \tag{1d}$$

The transition amplitude is given by[11]

$$\mathcal{T}_{ab} = \langle \psi_a^{(-)} | V_\beta | \phi_b \rangle = \langle \phi_a | V_\alpha | \psi_b^{(+)} \rangle . \tag{2}$$

This transition amplitude will be an element of the T matrix or the K matrix depending on whether the Green's function operators G_α, G_β, ... etc., are required to fulfill outgoing or standing wave asymptotic boundary conditions.

In the original two-body formalism of Lippmann and Schwinger[1] and in the many-body formalism of Hüfner and Lemmer[4] it is assumed that only one partition, say α, need be considered. Then the variational function for the transition amplitude is taken to be[11]

$$\hat{\mathcal{T}}_{aa'} = \frac{\langle \phi_a | V_\alpha | \hat{\psi}_{a'}^{(+)} \rangle \langle \hat{\psi}_a^{(-)} | V_\alpha | \phi_{a'} \rangle}{\langle \hat{\psi}_a^{(-)} | V_\alpha (1 - G_\alpha V_\alpha) | \hat{\psi}_{a'}^{(+)} \rangle} . \tag{3}$$

It can be readily verified that $\delta \hat{\mathcal{T}}_{aa'} / \delta \hat{\psi}_{a'}^{(+)} = 0$ and $\delta \hat{\mathcal{T}}_{aa'} / \delta \hat{\psi}_a^{(-)} = 0$ when $\hat{\psi}_{a'}^{(+)} = \psi_{a'}^{(+)}$ and $\hat{\psi}_a^{(-)} = \psi_a^{(-)}$. In addition, setting $\hat{\psi}_{a'}^{(+)} = \psi_{a'}^{(+)}$ and $\hat{\psi}_a^{(-)} = \psi_a^{(-)}$ causes $\hat{\mathcal{T}}_{aa'}$ to become equal to $\mathcal{T}_{aa'}$.

We propose the generalization of the above variational principle that results from choosing the variational function to be

$$\hat{\mathcal{T}}_{ab} = \frac{\langle \phi_a | V_\alpha | \hat{\psi}_b^{(+)} \rangle \langle \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle}{\langle \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} | \hat{\psi}_b^{(+)} \rangle} , \tag{4}$$

where we have used the inverse of the wave matrix operator $\Omega_\beta^{(+)}$ defined by

$$\Omega_\beta^{(+)-1} = 1 - G_\beta V_\beta . \tag{5}$$

Consider first variation with respect to $\hat{\psi}_a^{(-)}$. The condition $\delta \hat{\mathcal{T}}_{ab} / \delta \hat{\psi}_a^{(-)} = 0$ implies

$$0 = \langle \delta \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle \langle \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} | \hat{\psi}_b^{(+)} \rangle - \langle \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle \langle \delta \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} | \hat{\psi}_b^{(+)} \rangle . \tag{6}$$

To fulfill this relationship for arbitrary $\delta \hat{\psi}_a^{(-)}$ it is sufficient that

$$V_\beta \phi_b = V_\beta \Omega_\beta^{(+)-1} \hat{\psi}_b^{(+)} \tag{7}$$

or $\hat{\psi}_b^{(+)} = \psi_b^{(+)}$ in the range of V_β.

Consider next variations with respect to $\hat{\psi}_b^{(+)}$. The condition $\delta \hat{\mathcal{T}}_{ab} / \delta \hat{\psi}_b^{(+)} = 0$ implies the following relationship:

$$0 = \langle \phi_a | V_\alpha | \delta \hat{\psi}_b^{(+)} \rangle \langle \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} | \hat{\psi}_b^{(+)} \rangle - \langle \phi_a | V_\alpha | \hat{\psi}_b^{(+)} \rangle \langle \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} | \delta \hat{\psi}_b^{(+)} \rangle . \tag{8}$$

This relation will hold for arbitrary $\delta \hat{\psi}_b^{(+)}$ if the function $\hat{\psi}_a^{(-)}$ is required to be a solution of

$$\langle \phi_a | V_\alpha = \langle \hat{\psi}_a^{(-)} | V_\beta \Omega_\beta^{(+)-1} . \tag{9}$$

This is not equivalent to requiring $\hat{\psi}_a^{(-)} = \psi_a^{(-)}$. From Eq. (1c) we can deduce

$$\langle \psi_a^{(-)} | \Omega_\alpha^{(-)\dagger -1} = \langle \psi_a^{(-)} | (1 - V_\alpha G_\alpha) = \langle \phi_a | . \tag{10}$$

Using this definition of the inverse of the wave matrix operator $\Omega_\alpha^{(-)}$, Eq. (9) can be rewritten in the form

$$\langle \phi_a | V_\alpha = \langle \hat{\psi}_\alpha^{(-)} | \Omega_\beta^{(-)\dagger -1} V_\beta . \tag{11}$$

Only for the case $\beta = \alpha$ is this relationship fulfilled by $\hat{\psi}_a^{(-)} = \psi_a^{(-)}$, corresponding to the single-partition version of the Schwinger variational principle.

We can see that if $\hat{\psi}_a^{(-)}$ is a solution of Eq. (9), then $\hat{\mathcal{T}}_{ab} = \langle \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle$. We must prove this to be equal to $\mathcal{T}_{ab} = \langle \psi_a^{(-)} | V_\beta | \phi_b \rangle$ or $\mathcal{T}_{ab} = \langle \phi_a | V_\alpha | \psi_b^{(+)} \rangle$. This is seen to be the case since Eq. (9) implies

$$\begin{aligned} \hat{\mathcal{T}}_{ab} = \langle \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle &= \langle \phi_a | V_\alpha (V_\beta \Omega_\beta^{(+)-1})^{-1} V_\beta | \phi_b \rangle \\ &= \langle \phi_a | V_\alpha \Omega_\beta^{(+)} | \phi_b \rangle \\ &= \langle \phi_a | V_\alpha | \psi_b^{(+)} \rangle = \mathcal{T}_{ab} . \end{aligned} \tag{12}$$

Our many-partition generalization of the Schwinger variational principle is thus endowed with the desired features. It yields a formalism which consists in having

$$\mathcal{T}_{ab} \simeq \frac{\langle \phi_a | V_\alpha | \hat{\psi}_b^{(+)} \rangle \langle \hat{\psi}_a^{(-)} | V_\beta | \phi_b \rangle}{\langle \hat{\psi}_a^{(-)} | V_\beta - V_\beta G_\beta V_\beta | \hat{\psi}_b^{(+)} \rangle} , \tag{13a}$$

where

$$\hat{\psi}_b^{(+)} \simeq \Gamma_\beta V_\beta \phi_b = \psi_b^{(+)} , \tag{13b}$$

$$\hat{\psi}_a^{(-)} \simeq \Gamma_\beta^\dagger V_\alpha^\dagger \phi_a , \tag{13c}$$

$$\Gamma_\beta = (V_\beta \Omega_\beta^{(+)-1})^{-1} = \Omega_\beta^{(+)} V_\beta^{-1} . \tag{13d}$$

We understand $\hat{\psi}_b^{(+)}$ and $\hat{\psi}_a^{(-)}$ to be approximate representations of the solutions of Eqs. (7) and (9), respectively.

At this point we differ from Hüfner and Lemmer[4] who propose the use of Eq. (13b) for $\hat{\psi}_b^{(+)}$ in Eq. (2) for $\mathcal{T}_{ab}$. By using the definition for $\mathcal{T}_{ab}$ shown in Eq. (2) instead of the variational expression shown in Eq. (13a), Hüfner and Lemmer, it seems to us, lose the benefit of the stationary property of the variational expression.

An alternative formulation of the variational principle uses the operator Γ_β rather than the wave functions $\psi_b^{(+)}$ and $\psi_a^{(-)}$ as the quantity to be varied. Substitution of Eqs. (13b) and (13c) into Eq. (13a) gives

$$\mathcal{T}_{ab} \simeq \frac{(\langle\phi_a | V_\alpha \hat{\Gamma}_\beta V_\beta | \phi_b\rangle)^2}{\langle\phi_a | V_\alpha \hat{\Gamma}_\beta (V_\beta - V_\beta G_\beta V_\beta)\hat{\Gamma}_\beta V_\beta | \phi_b\rangle}, \tag{14}$$

where $\hat{\Gamma}_\beta \simeq \Omega_\beta^{(+)} V_\beta^{-1}$ is the result of some approximate scheme of calculation. For instance, if we use a Hilbert space truncation method we would seek to approximate $\psi^{(\pm)}$ by

$$\hat{\psi}^{(\pm)} = \sum_1^{\mathfrak{N}} A_n^{(\pm)} \chi_n , \tag{15}$$

a finite state sum. The $A_n^{(\pm)}$'s would be determined with the help of Eqs. (13b) and (13c). The results would then be substituted into Eq. (13a). Equivalently, Γ_β could be approximated by

$$\hat{\Gamma}_\beta = \sum_m \sum_n |\chi_m\rangle (\hat{\Gamma}_\beta)_{mn} \langle\chi_n| , \tag{16a}$$

$$(\hat{\Gamma}_\beta)_{mn} = (M^{-1})_{mn} , \tag{16b}$$

$$M_{mn} = \langle\chi_m | V_\beta \Omega_\beta^{(+)-1} | \chi_n\rangle = \langle\chi_m | \Gamma_\beta^{-1} | \chi_n\rangle , \tag{16c}$$

where we used the truncated basis $\{\chi_n; n = 1, 2, \ldots, \mathfrak{N}\}$ to carry out an approximate inversion of $V_\beta \Omega_\beta^{(+)-1}$.

III. FULFILLING THE ASYMPTOTIC BOUNDARY CONDITIONS

From the definition of Eq. (5)

$$\begin{aligned}\Gamma_\beta &= \Omega_\beta^{(+)} V_\beta^{-1} \\ &= (1 - G_\beta V_\beta)^{-1} V_\beta^{-1} \\ &= (V_\beta - V_\beta G_\beta V_\beta)^{-1} .\end{aligned} \tag{17}$$

Thus it would appear that $V_\beta - V_\beta G_\beta V_\beta$ should be used for $V_\beta \Omega_\beta^{(+)-1}$ in Eq. (16c). This is appropriate for the single-partition case but not for the many-partition case. By inverting $V_\beta \Omega_\beta^{(+)-1}$ to secure a representation of Γ_β we are solving the equations of motion of the system. When Eq. (17) is used we are using the formal solution of the Lippmann-Schwinger equation[1] for the wave matrix operator

$$\Omega_\beta^{(+)} = 1 + G_\beta V_\beta \Omega_\beta^{(+)} \tag{18}$$

to represent that operator. For the many-partition case this characterization of the wave matrix operator is incomplete.[12] If the system admits of N distinct partitions, then the wave matrix will be a solution of N distinct integral equations. Let

$$\mathcal{G} = (E - H)^{-1} = (G_\alpha^{-1} - V_\alpha)^{-1} = (G_\beta^{-1} - V_\beta)^{-1} = \cdots \tag{19}$$

be the system Green's function operator. Then

$$\begin{aligned}\Omega_\beta^{(+)} &= (1 - G_\beta V_\beta)^{-1} = \mathcal{G} G_\beta^{-1} \\ &= G_\gamma G_\gamma^{-1} \mathcal{G} G_\beta^{-1} = G_\gamma (\mathcal{G}^{-1} + V_\gamma) \mathcal{G} G_\beta^{-1} \\ &= G_\gamma G_\beta^{-1} + G_\gamma V_\gamma \Omega_\beta^{(+)} \quad \gamma = 1, 2, \ldots, N .\end{aligned} \tag{20}$$

Each of these integral equations contains an asymptotic boundary condition constraint for $\Omega_\beta^{(+)}$ in a different region of configuration space. $\Omega_\beta^{(+)}$ must be a simultaneous solution of all these N equations.

It is easy to illustrate the difficulty if we replace Eq. (20) by

$$\Omega_\beta^{(+)} = \delta_{\gamma\beta} + G_\gamma V_\gamma \Omega_\beta^{(+)} .$$

This is justified in cases where we use $\Omega_\beta^{(+)}$ in expressions in which it operates on ϕ_β or approximations thereto. Then $\Omega_\alpha^{(+)}$ is the simultaneous solution of

$$\begin{aligned}\Omega_\alpha^{(+)} &= 1 + G_\alpha V_\alpha \Omega_\alpha^{(+)} \\ &= G_\beta V_\beta \Omega_\alpha^{(+)} \\ &= G_\gamma V_\gamma \Omega_\alpha^{(+)} \\ &\cdots\end{aligned}$$

while $\Omega_\beta^{(+)}$ is the simultaneous solution of

$$\begin{aligned}\Omega_\beta^{(+)} &= G_\alpha V_\alpha \Omega_\beta^{(+)} \\ &= 1 + G_\beta V_\beta \Omega_\beta^{(+)} \\ &= G_\gamma V_\gamma \Omega_\beta^{(+)} \\ &\cdots ,\end{aligned}$$

and so on. We see that the equation

$$\Omega = 1 + G_\alpha V_\alpha \Omega$$

has the solution $\Omega_\alpha^{(+)} + b\Omega_\beta^{(+)} + c\Omega_\gamma^{(+)} + \cdots$ with arbitrary constants b, c, $\ldots$. Thus a single equation of the set does not have a unique solution.

To construct a formal simultaneous solution of the N integral equations shown in Eq. (20) it is convenient to start by forming N independent linear combinations of these equations.

$$\Omega_\beta^{(+)} = \sum_{\gamma=1}^{N} W_{\alpha\gamma} G_\gamma G_\beta^{-1} + \sum_{\gamma=1}^{N} W_{\alpha\gamma} G_\gamma V_\gamma \Omega_\beta^{(+)} \qquad \alpha = 1, 2, \ldots, N, \tag{21a}$$

$$\sum_{\gamma=1}^{N} W_{\alpha\gamma} = 1 . \tag{21b}$$

The numerical coefficients $W_{\alpha\gamma}$ are arbitrary except for the requirement that the N equations contained in Eq. (21a) be independent and except for the constraint contained in Eq. (21b). Next operate on Eq. (21a) with V_α.

$$V_\alpha \Omega_\beta^{(+)} = \sum_{\gamma=1}^{N} V_\alpha W_{\alpha\gamma} G_\gamma G_\beta^{-1} + \sum_{\gamma=1}^{N} V_\alpha W_{\alpha\gamma} G_\gamma V_\gamma \Omega_\beta^{(+)} . \qquad (22)$$

This is the Kouri-Levin equation[8] for the transition operator. In matrix notation it reads

$$T = QUG^{-1} + QT , \qquad (23a)$$

$$T_{\alpha\beta} = V_\alpha \Omega_\beta^{(+)} , \qquad (23b)$$

$$Q_{\alpha\beta} = V_\alpha W_{\alpha\beta} G_\beta . \qquad (23c)$$

$$U_{\alpha\beta} = 1 , \qquad (24a)$$

$$(G^{-1})_{\alpha\beta} = G_\alpha^{-1} \delta_{\alpha\beta} . \qquad (24b)$$

Its formal solution is

$$T = (1 - Q)^{-1} QUG^{-1} . \qquad (25)$$

From the formal solution we find

$$\Gamma_\beta = V_\alpha^{-1} T_{\alpha\beta} V_\beta^{-1}$$

$$= \sum_{\gamma=1}^{N} [(V - QV)^{-1} Q]_{\alpha\gamma} G_\beta^{-1} V_\beta^{-1} . \qquad (26)$$

An alternative expression for Γ_β is found via the following sequence of steps which are parallel to those leading from Eq. (20) to Eq. (26).

$$\Omega_\beta^{(+)} = \mathcal{G} G_\beta^{-1} = \mathcal{G}(\mathcal{G}^{-1} + V_\beta)$$

$$= 1 + \mathcal{G} V_\beta = 1 + \Omega_\gamma^{(+)} G_\gamma V_\beta , \qquad (27)$$

$$\Omega_\beta^{(+)} = 1 + \sum_{\gamma=1}^{N} \Omega_\gamma^{(+)} G_\gamma W_{\gamma\beta} V_\beta , \qquad (28a)$$

$$\sum_{\gamma=1}^{N} W_{\gamma\beta} = 1 , \qquad (28b)$$

$$T_{\alpha\beta} = V_\alpha + \sum_{\gamma=1}^{N} T_{\alpha\gamma} G_\gamma W_{\gamma\beta} V_\beta . \qquad (29)$$

Equation (29) is very closely related to one given by Baer and Kouri.[7]

$$T = VU + TP , \qquad (30a)$$

$$P_{\alpha\beta} = G_\alpha W_{\alpha\beta} V_\beta , \qquad (30b)$$

$$V_{\alpha\beta} = V_\alpha \delta_{\alpha\beta} , \qquad (30c)$$

$$T = VU(1 - P)^{-1} , \qquad (31)$$

$$\Gamma_\beta = \sum_{\gamma=1}^{N} [(V - VP)^{-1}]_{\gamma\beta} . \qquad (32)$$

The single-partition result is recovered by setting $N = 1$ and $W_{\beta\beta} = 1$.

Equations (26) and (32) represent many-partition generalizations of Eq. (17) which incorporate the full set of asymptotic boundary conditions.

IV. SUPPRESSION OF DISCONNECTED GRAPHS

It thus seems advisable to use Eq. (26) or Eq. (32) for Γ_β in the construction of $\hat{\Gamma}_\beta$ via Eq. (16) for use in calculating the transition amplitude ${}_{ab}$ by means of Eq. (14). In using Eq. (32) for Γ_β in Eq. (16) for $\hat{\Gamma}_\beta$, we are generating an approximate solution of the integral equation displayed in Eq. (28) by use of a finite basis of states. We can be sure that this procedure converges to the correct result in the limit that the dimension of the basis becomes very large if the kernel of the integral equation is completely continuous.[13] The kernel of our equation will be completely continuous if the iteration series expansion of the integral equation is such that beyond some finite order all terms of the expansion have connected graphs.[14]

The kernel of Eq. (28) is $GWV = P$. We have noted that the constraints on the coefficients $W_{\alpha\beta}$ are not very restrictive. By virtue of the fact that the subscripts of $W_{\alpha\beta}$ serve to identify different partitions of the system into two clusters and since V_α represents the entire intercluster interaction for partition α, it is easy to see how we may use the freedom we have in choosing the elements $W_{\alpha\beta}$ to prevent the appearance of infinite sets of disconnected graphs in the iteration expansion of Eq. (28).

One way to do this[9] is to choose the $W_{\alpha\beta}$'s so that the operators V_α that appear in any term of the iteration expansion always appear in a particular sequence and that this sequence contains all possible partitions. Then there can never by any graph of order higher than N for which a group of particles has only mutual interactions since that graph must of necessity contain V_γ where γ is the partition for which that group of particles is one of the two clusters. For example, we can choose

$$W_{\alpha,\alpha+1} = 1 \quad \alpha = 1, 2, \ldots, N-1 , \qquad (33a)$$

$$W_{N,1} = 1 \qquad (33b)$$

$$\text{all other } W_{\alpha\beta} = 0 , \qquad (33c)$$

where N is the total number of distinct partitions possible for the many-body system.

Use of the above choice for W causes the operators Q^N and P^N to be diagonal in partition space. This fact suggests the use of an alternative expression for Γ_β in place of Eq. (26) or (32). For example Eq. (32) can be transformed in the following manner:

$$\Gamma_\beta = \sum_{\gamma=1}^{N} [(1-P)^{-1}]_{\gamma\beta} V_\beta^{-1}$$
$$= \sum_{\gamma=1}^{N} [(1-P)^{-1}(1-P^N)(1-P^N)^{-1}]_{\gamma\beta} V_\beta^{-1}$$
$$= \sum_{\gamma=1}^{N} \{ \delta_{\gamma\beta} + P_{\gamma\beta} + (P^2)_{\gamma\beta} + \cdots + (P^{N-1})_{\gamma\beta}\} \times [V_\beta - V_\beta (P^N)_{\beta\beta}]^{-1}$$
$$= \{1 + P_{\beta-1,\beta} + (P^2)_{\beta-2,\beta} + \cdots + (P^{N-1})_{\beta+1,\beta}\} \times [V_\beta - V_\beta(P^N)_{\beta\beta}]^{-1}. \quad (34)$$

A similar transformation can be performed for Eq. (26). In the equation above the operator to be inverted is diagonal in partition space so that the dimension of the matrix to be inverted is reduced by a factor N. That brings the dimension back to the dimension $\mathfrak{N}$ of the space in which $V_\beta - V_\beta G_\beta V_\beta$ is to be inverted in the single-partition case. Thus, in place of Eq. (16) we would have

$$\hat{\Gamma}_\beta = \{1 + P_{\beta-1,\beta} + (P^2)_{\beta-2,\beta} + \cdots + (P^{N-1})_{\beta+1,\beta}\} M_\beta , \quad (35a)$$

$$M_\beta = \sum_m \sum_n |\chi_m\rangle M_{mn} \langle \chi_n | , \quad (35b)$$

$$M_{mn} = (N^{-1})_{mn} , \quad (35c)$$

$$N_{mn} = \langle \chi_m | V_\beta - V_\beta (P^N)_{\beta\beta} | \chi_n \rangle . \quad (35d)$$

V. KOHN VARIATIONAL PRINCIPLE

For some cases the Born approximation to the transition amplitude provides a fair approximation. In such cases it might be advantageous to use a variational function to approximate the difference between the exact transition amplitude and its first order approximation. The method appropriate to this task is the Kohn variational principle.[2] We will sketch out below a manner in which the Kohn variational principle may be generalized for use with the many-body problem which is similar to our treatment of the Schwinger variational principle.

The Kohn variational function for the transition amplitude is

$$\tilde{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \tilde{\psi}_b^{(+)} \rangle + \langle \tilde{\psi}_a^{(-)} | E - H | \tilde{\psi}_B^{(+)} \rangle . \quad (36)$$

This functional has the disadvantage that it is sensitive to the asymptotic behavior of the trial wave functions $\tilde{\psi}_a^{(-)}$ and $\tilde{\psi}_b^{(+)}$. A slight alteration can remedy this problem.

$$\hat{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \tilde{\psi}_b^{(+)} \rangle - \langle \hat{\psi}_a^{(-)} - \phi_a | E - H | \tilde{\psi}_b^{(+)} \rangle . \quad (37)$$

The trial wave functions are assumed to have the forms

$$\hat{\psi}_b^{(+)} = \phi_b + \hat{\chi}_b^{(+)} \quad (38a)$$
$$= \phi_b + \hat{\mathcal{G}} V_\beta \phi_b , \quad (38b)$$
$$\hat{\psi}_a^{(-)} = \phi_a + \hat{\chi}_a^{(-)} \quad (39a)$$
$$= \phi_a + \hat{\mathcal{G}}^\dagger V_\alpha^\dagger \phi_a . \quad (39b)$$

Substituting these forms back into the variational function gives

$$\hat{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \phi_b \rangle + \langle \phi_a | V_\alpha | \hat{\chi}_b^{(+)} \rangle + \langle \hat{\chi}_a^{(+)} | V_\beta | \phi_b \rangle - \langle \hat{\chi}_a^{(+)} | E - H | \hat{\chi}_b^{(+)} \rangle \quad (40a)$$
$$= \langle \phi_a | V_\alpha | \phi_b \rangle + 2 \langle \phi_a | V_\alpha \hat{\mathcal{G}} V_\beta | \phi_b \rangle - \langle \phi_\alpha | V_\alpha \hat{\mathcal{G}} (E - H) \hat{\mathcal{G}} V_\beta | \phi_b \rangle . \quad (40b)$$

An alternative to the above expressions which is independent of the normalization of the trial wave functions $\hat{\chi}^{(\pm)}$ is

$$\hat{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \phi_b \rangle + \frac{\langle \phi_a | V_\alpha | \hat{\chi}_b^{(+)} \rangle \langle \hat{\chi}_a^{(+)} | V_\beta | \phi_b \rangle}{\langle \hat{\chi}_a^{(+)} | E - H | \hat{\chi}_b^{(+)} \rangle} \quad (41a)$$
$$= \langle \phi_a | V_\alpha | \phi_b \rangle + \frac{(\langle \phi_a | V_\alpha \hat{\mathcal{G}} V_\beta | \phi_b \rangle)^2}{\langle \phi_a | V_\alpha \hat{\mathcal{G}} (E - H) \hat{\mathcal{G}} V_\beta | \phi_b \rangle} . \quad (41b)$$

Inasmuch as $\mathcal{G} = \Omega_\beta^{(+)} G_\beta = \Gamma_\beta V_\beta G_\beta$, we can write the Kohn variational function in terms of the same operator Γ_β as was used in the Schwinger variational function.

$$\hat{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \phi_b \rangle + \frac{(\langle \phi_a | V_\alpha \hat{\Gamma}_\beta V_\beta G_\beta V_\beta | \phi_b \rangle)^2}{\langle \phi_a | V_\alpha \hat{\Gamma}_\beta (V_\beta - V_\beta G_\beta V_\beta) \hat{\Gamma}_\beta V_\beta G_\beta V_\beta | \phi_b \rangle} . \quad (42)$$

Again the use of something like Eq. (35) to construct a representation for $\hat{\Gamma}_\beta$ would be indicated.

VI. USEFUL EXPLICIT EXPRESSIONS FOR THE VARIATIONAL FUNCTIONS AND THE TRANSITION AMPLITUDE

We have noted in Sec. IV that the choice for W given in Eq. (33) causes the operators Q^N and P^N to be diagonal in partition space. This fact was used to derive Eq. (34) from Eq. (32). Let us now carry out a similar transformation on Eq. (25) to get an alternative expression for the operator Γ_β:

$$T_{\alpha\beta} = V_\alpha \Gamma_\beta V_\beta = \sum_{\gamma=1}^{N} [(1-Q)^{-1} Q]_{\alpha\gamma} G_\beta^{-1}$$
$$= \sum_{\gamma=1}^{N} [(1-Q^N)^{-1}(1-Q^N)(1-Q)^{-1} Q]_{\alpha\gamma} G_\beta^{-1}$$
$$= V_\alpha [V_\alpha - (Q^N)_{\alpha\alpha} V_\alpha]^{-1} \times \sum_{\gamma=1}^{N} (Q + Q^2 + \cdots + Q^N)_{\alpha\gamma} G_\beta^{-1}$$
$$= V_\alpha [V_\alpha - (Q^N)_{\alpha\alpha} V_\alpha]^{-1} [Q_{\alpha,\alpha+1} + (Q^2)_{\alpha,\alpha+2} + \cdots + (Q^N)_{\alpha,\alpha}] G_\beta^{-1} . \quad (43)$$

When $T_{\alpha\beta}$ operates on ϕ_b it will give zero unless the $G_\beta{}^{-1}$ factor is immediately preceded by a factor G_β. Then the $(Q^{n(\alpha,\beta)})_{\alpha,\beta}$ term is the only one which gives a nonzero result, where $n(\alpha,\beta)=\beta-\alpha$ modulo N except that $n(\alpha,\alpha)=N$.

$$T_{\alpha\beta}|\phi_b\rangle = V_\alpha(V_\alpha - V_\alpha^{(+)}G_\alpha V_\alpha)^{-1}V_{\alpha\beta}^{(+)}|\phi_b\rangle . \quad (44a)$$

$$V_\alpha^{(+)} = (Q^N G^{-1})_{\alpha\alpha} = V_\alpha G_{\alpha+1}V_{\alpha+1}V_{\alpha+2}\cdots G_{\alpha-1}V_{\alpha-1} . \quad (44b)$$

$$V_{\alpha\beta}^{(+)} = (Q^{n(\alpha,\beta)}G^{-1})_{\alpha\beta} = V_\alpha G_{\alpha+1}V_{\alpha+1}G_{\alpha+2}\cdots G_{\beta-1}V_{\beta-1} . \quad (44c)$$

The quantity $\hat{\Gamma}_\beta V_\beta|\phi_b\rangle$ appears in the Schwinger variational function, but in the Kohn variational function the quantity $\hat{\Gamma}_\beta V_\beta G_\beta V_\beta|\phi_b\rangle$ appears instead. However, this can be replaced by $G_\beta V_\beta \hat{\Gamma}_\beta V_\beta|\phi_b\rangle$ by virtue of the fact that

$$\Gamma_\beta V_\beta G_\beta = \mathcal{G} = G_\beta V_\beta \Gamma_\beta . \quad (45)$$

In both variational functions the quantity $\langle\phi_a|V_\alpha\hat{\Gamma}_\beta$ appears. This quantity is also susceptable to a similar kind of simplification. For this purpose we consider the following representation for the operator Γ_β:

$$\Gamma_\beta = V_\beta{}^{-1}T_{\beta\alpha}^{(-)}V_\alpha{}^{-1} , \quad (46a)$$

$$T_{\beta\alpha}^{(-)} = \Omega_\beta^{(-)\dagger}V_\alpha = (1 - V_\beta G_\beta)^{-1}V_\alpha = G_\beta{}^{-1}\mathcal{G}V_\alpha . \quad (46b)$$

The operator $T_{\beta\alpha}^{(-)}$ can be shown to fulfill a set of coupled integral equations similar to those fulfilled by the $T_{\beta\alpha}$.

$$T^{(-)} = G^{-1}UP + T^{(-)}P = G^{-1}UP(1-P)^{-1} . \quad (47)$$

The quantities G^{-1}, U, and P are defined in Eqs. (24) and (30). Proceeding as we did in the derivation of Eqs. (34) and (43) we find

$$\begin{aligned} T_{\beta\alpha}^{(-)} &= V_\beta\Gamma_\beta V_\alpha = G_\beta{}^{-1}\sum_{\gamma=1}^{N}\{P(1-P)\}_{\gamma\alpha} \\ &= G_\beta{}^{-1}\sum_{\gamma=1}^{N}\{P(1-P)^{-1}(1-P^N)(1-P^N)^{-1}V^{-1}\}_{\gamma\alpha}V_\alpha \\ &= G_\beta{}^{-1}\sum_{\gamma=1}^{N}[P+P^2+\cdots+P^N]_{\gamma\alpha} \times[V_\alpha-(VP^N)_{\alpha\alpha}]^{-1}V_\alpha \\ &= G_\beta{}^{-1}[P_{\alpha-1,\alpha}+(P^2)_{\alpha-2,\alpha}+\cdots+(P^N)_{\alpha,\alpha} \times[V_\alpha-(VP^N)_{\alpha\alpha}]^{-1}V_\alpha . \end{aligned} \quad (48)$$

Now in both the Schwinger and Kohn variational functions we see

$$\begin{aligned} \langle\phi_a|V_\alpha\hat{\Gamma}_\beta(V_\beta - V_\beta G_\beta V_\beta) &= \langle\phi_a|V_\alpha\hat{\Gamma}_\beta V_\beta G_\beta(G_\beta{}^{-1}-V_\beta) \\ &= \langle\phi_a|V_\alpha\hat{\mathcal{G}}\mathcal{G}^{-1} = \langle\phi_a|V_\alpha\hat{\Gamma}_\alpha V_\alpha G_\alpha(G_\alpha{}^{-1}-V_\alpha) \\ &= \langle\phi_a|V_\alpha\hat{\Gamma}_\alpha(V_\alpha - V_\alpha G_\alpha V_\alpha) . \end{aligned} \quad (49)$$

If Eq. (48) is used in Eq. (49), the action of $G_\alpha{}^{-1}$ on ϕ_a will cause all terms except $(P^N)_{\alpha,\alpha}$ to give zero contributions. Thus we find

$$\langle\phi_a|V_\alpha\Gamma_\beta(V_\beta - V_\beta G_\beta V_\beta) = \langle\phi_a|V_\alpha^{(-)}(V_\alpha - V_\alpha G_\alpha V_\alpha^{(-)})^{-1}(V_\alpha - V_\alpha G_\alpha V_\alpha) \quad (50a)$$

$$V_\alpha^{(-)} = (G^{-1}P^N)_{\alpha\alpha} = V_{\alpha+1}G_{\alpha+1}V_{\alpha+2}\cdots V_{\alpha-1}G_{\alpha-1}V_\alpha . \quad (50b)$$

Let us define

$$\Gamma_\beta^{(+)} = (V_\beta - V_\beta^{(+)}G_\beta V_\beta)^{-1} , \quad (51a)$$

$$\Gamma_\alpha^{(-)} = (V_\alpha - V_\alpha G_\alpha V_\alpha^{(-)})^{-1} . \quad (51b)$$

Then we can use the results derived above to yield the following explicit expressions: The transition amplitude can be written

$$\mathcal{T}_{ab} = \langle\phi_a|V_\alpha\Gamma_\beta V_\beta|\phi_b\rangle = \langle\phi_a|V_\alpha\Gamma_\alpha^{(+)}V_{\alpha\beta}^{(+)}|\phi_b\rangle . \quad (52)$$

Alternatively,

$$\mathcal{T}_{ab} = \langle\phi_a|V_\alpha + V_\alpha\Gamma_\beta V_\beta G_\beta V_\beta|\phi_b\rangle = \langle\phi_a|V_\alpha + V_\alpha G_\beta V_\beta\Gamma_\beta^{(+)}V_\beta^{(+)}|\phi_b\rangle . \quad (53)$$

The Schwinger variational function can be written

$$\hat{\mathcal{T}}_{ab} = \frac{(\langle\phi_a|V_\alpha\hat{\Gamma}_\alpha^{(+)}V_{\alpha\beta}^{(+)}|\phi_b\rangle)^2}{\langle\phi_a|V_\alpha^{(-)}\hat{\Gamma}_\alpha^{(-)}(V_\alpha - V_\alpha G_\alpha V_\alpha)\hat{\Gamma}_\beta^{(+)}V_\beta^{(+)}|\phi_b\rangle} \quad (54)$$

and the Kohn variational function can be written

$$\hat{\mathcal{T}}_{ab} = \langle\phi_b|V_\alpha|\phi_b\rangle + \frac{(\langle\phi_a|V_\alpha G_\beta V_\beta\hat{\Gamma}_\beta^{(+)}V_\beta^{(+)}|\phi_b\rangle)^2}{\langle\phi_a|V_\alpha^{(-)}\hat{\Gamma}_\alpha^{(-)}(V_\alpha - V_\alpha G_\alpha V_\alpha)G_\beta V_\beta\hat{\Gamma}_\beta^{(+)}V_\beta^{(+)}|\phi_b\rangle} . \quad (55)$$

The expressions shown above are well suited to calculations based on the evaluation of $\Gamma_\beta^{(+)}$ and $\Gamma_\alpha^{(-)}$ by means of inversion in a truncated basis. Another approach would be the approximate solution of integral equations. Quantities related to

$\Gamma_\alpha^{(\pm)}$ which fulfill convenient integral equations are

$$\Gamma_\beta^{(+)} V_{\beta\alpha}^{(+)} = \omega_{\beta\alpha}^{(+)} = V_\beta^{-1} V_{\beta\alpha}^{(+)} + V_\beta^{-1} V_\beta^{(+)} G_\beta V_\beta \omega_{\beta\alpha}^{(+)}, \tag{56a}$$

$$V_\alpha^{(-)} \Gamma_\alpha^{(-)} = \omega_\alpha^{(-)} = V_\alpha^{(-)} V_\alpha^{-1} + \omega_\alpha^{(-)} V_\alpha G_\alpha V_\alpha^{(-)} V_\alpha^{-1}, \tag{56b}$$

$$V_\beta \omega_{\beta\alpha}^{(+)} = T_{\beta\alpha}^{(+)} = V_{\beta\alpha}^{(+)} + V_\beta^{(+)} G_\beta T_{\beta\alpha}^{(+)}, \tag{57a}$$

$$\omega_\alpha^{(-)} V_\alpha = T_\alpha^{(-)} = V_\alpha^{(-)} + T_\alpha^{(-)} G_\alpha V_\alpha^{(-)}. \tag{57b}$$

Rewriting our expressions for the transition amplitude in terms of these quantities gives

$$\mathcal{T}_{ab} = \langle \phi_a | V_\alpha \omega_{\alpha\beta}^{(+)} | \phi_b \rangle \tag{58a}$$

$$= \langle \phi_a | V_\alpha + V_\alpha G_\beta T_\beta^{(+)} | \phi_b \rangle, \tag{58b}$$

$$\hat{\mathcal{T}}_{ab} = \frac{(\langle \phi_a | V_\alpha \hat{\omega}_{\alpha\beta}^{(+)} | \phi_b \rangle)^2}{\langle \phi_a | \hat{\omega}_\alpha^{(-)} (V_\alpha - V_\alpha G_\alpha V_\alpha) \hat{\omega}_\beta^{(+)} | \phi_b \rangle}, \tag{59}$$

$$\hat{\mathcal{T}}_{ab} = \langle \phi_a | V_\alpha | \phi_b \rangle + \frac{(\langle \phi_a | V_\alpha G_\beta \hat{T}_\beta^{(+)} | \phi_b \rangle)^2}{\langle \phi_a | \hat{T}_\alpha^{(-)} (1 - G_\alpha V_\alpha) G_\beta \hat{T}_\beta^{(+)} | \phi_b \rangle}. \tag{60}$$

VII. SUMMARY

It is demonstrated that the Schwinger variational principle can be generalized so that it may be applied to a many-body system with open rearrangement channels. A variational expression for the transition amplitude $\mathcal{T}_{ab}$ in terms of the operator $\Gamma_\beta = \Omega_\beta^{(+)} V_\beta^{-1}$ is given. An approximate representation for Γ_β is to be used in the variational expression to produce an approximation to $\mathcal{T}_{ab}$. The evaluation of $\Gamma_\beta = V_\alpha^{-1} T_{\alpha\beta} V_\beta^{-1}$ corresponds to the solution of a set of integral equations for the $T_{\alpha\beta}$ These equations contain a set of fairly arbitrary parameters $W_{\alpha\beta}$. By appropriate choice of the parameters $W_{\alpha\beta}$ the kernel of this set of integral equations becomes completely continuous so that we are assured that an approximate evaluation of Γ_β can be a member of a convergent sequence of approximations.

Finally, it is shown that the same ideas can be used to generalize the Kohn variational principle to the many-body case.

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