Equivalent Hamiltonians

W. N. Polyzou*
Department of Physics and Astronomy, The University of Iowa, Iowa City, IA 52242
(Dated: June 24, 2010)

I give a characterization of the conditions for two Hamiltonians to be equivalent, discuss the construction of the operators that relate equivalent Hamiltonians, and introduce variational methods that can select Hamiltonians with desirable features from the space of equivalent Hamiltonians.

PACS numbers: 21.45.Ff,13.75.Cs,03.65.Nk

I. INTRODUCTION

In this paper I study the freedom available to redefine interactions without changing the scattering and bound-state observables of a quantum mechanical system. I consider how this freedom can be used to formulate interactions that have advantages in various situations. The Hamiltonians discussed in this paper are equivalent in the mathematical sense at all energy scales; this a stronger requirement than the more flexible notion of equivalence used in effective field theory that only requires equivalence up to some order in the expansion parameter. Even with this more restrictive notion of equivalence there is a very large class of equivalent Hamiltonians.

There are a number of formal methods that start from a set of high-quality two and three-body interactions and construct an equivalent set of interactions that fit the same bound-state and scattering data. These include renormalization group methods and methods based on specific unitary transformations that block diagonalize Hamiltonians [1][2] [3] [4] [5][6]. The compelling feature of all of these methods is that the off-diagonal matrix elements that couple the high- and low-energy parts of the problem are suppressed in the transformed interactions. This leads to a low-energy effective theories that are approximately decoupled from the high-energy part of the problem. This has computational advantages in many-body calculations. The price paid is that the transformed Hamiltonian has new many-body forces involving any number of particles. This is similar to what is observed using field redefinitions in effective field theories, although the transformed theories discussed in this paper are in principle equivalent to the original theories for all energies.

In this paper I introduce a method that can be used to provide independent control of the two, three, and many-body interactions. Much of the work contained in this paper has been discussed in [7]. The approach is to start with the general class of equivalent interactions. This is then restricted to a subset that can be treated variationally. Positive functionals are introduced that have minimum values for equivalent potentials with selected properties. For example it is possible to design functionals that select models where the dynamics for energies above some given scale approximately decouples from the dynamics for energies below some scale, models that have weak three and four-body interactions or models that emphasize an approximate symmetry.

II. MULTICHANNEL SCATTERING THEORY

In this section I give a brief summary of multichannel scattering theory that is relevant for this work.

The Hilbert space, $\mathcal{H}_1$, for a single particle of mass m and spin j is the space of square integrable functions of particle's linear momentum and magnetic quantum number

$$\langle \mathbf{p},\mu|\psi\rangle = \psi(\mathbf{p},\mu) \qquad \langle\psi|\psi\rangle = \int d\mathbf{p} \sum_{\mu=-j}^{j} |\psi(\mathbf{p},\mu)|^2 < \infty. \tag{2.1}$$

The N-particle Hilbert space is the N-fold tensor product of single-particle Hilbert spaces

$$\mathcal{H} := \otimes_{i=1}^{N} \mathcal{H}_i. \tag{2.2}$$

* This work supported in part by the U.S. Department of Energy, under contract DE-FG02-86ER40286

The total linear momentum and total Galilean mass of the N-particle system are the multiplication operators

$$\mathbf{p} := \sum_{i=1}^{N} \mathbf{p}_i \qquad M = \sum_{i=1}^{N} m_i. \tag{2.3}$$

The N-body Hamiltonian H has a N-body bound state if the center-of-mass Hamiltonian,

$$h := H - \frac{\mathbf{p}^2}{2M}, \tag{2.4}$$

has a discrete eigenvalue, $-\epsilon$. If the Hamiltonian is rotationally and translationally invariant it is possible to find simultaneous eigenstates of h, $\mathbf{p}$, the total N-body spin and the projection of the total N-body spin on the 3-axis. I denote these eigenstates by $|(\epsilon_i, j_i), \mathbf{p}, \mu\rangle$, where the index i labels different bound states when h has more than one bound state.

To define scattering channels let a denote a partition of the N- particles into n_a disjoint non-empty clusters of n_{a_i} particles. There is a scattering channel α associated with the partition a if there is a n_{a_i}-body bound state in each of the n_a clusters of the partition a. Channel states asymptotically look like a collection of n_a mutually non-interacting bound clusters.

The direct product of the n_a bound states in the channel α_i

$$\Phi_{\alpha_i} = |(\epsilon_1, j_1), \mathbf{p}_1, \mu_1\rangle \times \cdots \times |(\epsilon_{n_a}, j_{n_a}), \mathbf{p}_{n_a}, \mu_{n_a}\rangle \tag{2.5}$$

defines the mapping Φ_{α_i}, called the channel injection operator, from the channel Hilbert space, $\mathcal{H}_{\alpha_i}$, which is tensor product of n_a single particle Hilbert spaces,

$$\mathcal{H}_{\alpha_i} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{n_a} \tag{2.6}$$

to the N-particle Hilbert space by

$$\Phi_{\alpha_i}|\mathbf{f}_{\alpha_i}\rangle = \int \sum_{\mu_a \cdots \mu_{n_a}} |(h_1, j_1), \mathbf{p}_1, \mu_1\rangle \times \cdots \times |(h_{n_a}, j_{n_a}), \mathbf{p}_{n_a}, \mu_{n_a}\rangle \times$$

$$f_1(\mathbf{p}_1, \mu_1) \cdots f_{n_a}(\mathbf{p}_{n_a}, \mu_{n_a}) \prod d\mathbf{p}_i \tag{2.7}$$

where $f_j(\mathbf{p}_j, \mu_j)$ are wave packets describing the momentum and spin distribution of the jth asymptotically bound cluster.

The asymptotic Hilbert space, $\mathcal{H}_f$, is the direct sum of all of the channel Hilbert spaces, *including* the one-cluster channels that correspond to N-particle bound states,

$$\mathcal{H}_f = \oplus_i \mathcal{H}_{\alpha_i}, \tag{2.8}$$

and the multichannel injection operator $\Phi : \mathcal{H}_f \to \mathcal{H}$ is

$$\Phi|\mathbf{f}\rangle := \sum_i \Phi_{\alpha_i}|\mathbf{f}_{\alpha_i}\rangle \tag{2.9}$$

where

$$|\mathbf{f}\rangle = \oplus_{\alpha_i}|\mathbf{f}_{\alpha_i}\rangle. \tag{2.10}$$

For each partition a there may be 0, 1 or a finite number of channels.

The unitary time evolution operator $U_{\alpha_i}(t)$ on each channel subspace, $\mathcal{H}_{\alpha_k}$ is

$$U_{\alpha_k}(t) = e^{-i\sum_j(\mathbf{p}_j^2/2m_j - \epsilon_j)t} \tag{2.11}$$

where $\mathbf{p}_j$ is the total momentum of the j-th bound cluster in the channel α_k, m_j is the total mass of the j-th bound cluster of channel α_k and $-\epsilon_j$ is the binding energy of the j-th bound cluster of channel α_i.

The asymptotic time-evolution operator on $\mathcal{H}_f$ is the direct sum of the channel time-evolution operators

$$U_f(t) = \oplus_i U_{\alpha_i}(t). \tag{2.12}$$

The asymptotic Hamiltonian, H_f, is the infinitesimal generator of $U_f(t)$. Multichannel Møller wave operators

$$\Omega_\pm : \mathcal{H}_f \to \mathcal{H} \tag{2.13}$$

are defined by the strong limits

$$\Omega_\pm = \lim_{t\to\pm\infty} U(-t)\Phi U_f(t) \tag{2.14}$$

where $U(t) = e^{-iHt}$ is the time evolution operator on $\mathcal{H}$. The multichannel scattering operator $S : \mathcal{H}_f \to \mathcal{H}_f$, is defined by

$$S = \Omega_+^\dagger \Omega_-. \tag{2.15}$$

In order to indicate the dependence of the wave operator $\Omega_\pm$ on H, H_f and Φ I use the notation

$$\Omega_\pm = \Omega_\pm(H, \Phi, H_f) \qquad S(H, \Phi, H_f) = \Omega_+^\dagger(H, \Phi, H_f)\Omega_-(H, \Phi, H_f). \tag{2.16}$$

I say that the scattering theory is asymptotically complete if the wave operators satisfy the following completeness relations:

$$I_{\mathcal{H}} = \Omega_+(H, \Phi, H_f)\Omega_+^\dagger(H, \Phi, H_f) = \Omega_-(H, \Phi, H_f)\Omega_-^\dagger(H, \Phi, H_f) \tag{2.17}$$

and

$$I_{\mathcal{H}_f} = \Omega_+^\dagger(H, \Phi, H_f)\Omega_+(H, \Phi, H_f) = \Omega_-^\dagger(H, \Phi, H_f)\Omega_-(H, \Phi, H_f). \tag{2.18}$$

where $I_{\mathcal{H}}$ and $I_{\mathcal{H}_f}$ are the identity operators on $\mathcal{H}$ and $\mathcal{H}_f$ respectively.

The intertwining relations,

$$H\Omega_\pm(H, \Phi, H_f) = \Omega_\pm(H, \Phi, H_f)H_f, \tag{2.19}$$

follow directly from the definition (2.14) and lead to energy conservation,

$$[H_f, S]_- = 0, \tag{2.20}$$

in the scattering operator.

In all that follows the wave operators are assumed to exist and satisfy the completeness relations (2.17) and (2.18). The two-Hilbert space formulation of multichannel scattering theory summarized above is equivalent to the standard formulation of multichannel scattering. It has the advantage that the notation allows all channels to be treated simultaneously.

III. CLUSTER EXPANSIONS

In this section I introduce combinatorial methods to treat cluster expansions in this work[8][9][10]. These provide an efficient notation for computing the many-body interactions that appear in different equivalent Hamiltonians.

I begin by introducing a useful notation. I let $\mathcal{P}$ denote the set of partitions of N particles into disjoint, non-empty clusters. I use lower case Latin letters, a, to denote partitions of N particles, n_a to denote the number of clusters in the partition a, and n_{a_i} to denote the number of particles in the ith cluster of the partition a:

$$N = \sum_{i=1}^{n_a} n_{a_i}. \tag{3.1}$$

Thus $a = (125)(37)(64)$ is a three-cluster partition of seven particles, with one three-particle cluster and two two-particle clusters.

There is a natural partial ordering on the set of partitions of N particles given by

$$a \subseteq b \quad \text{or} \quad b \supseteq a \tag{3.2}$$

if every particle in the same cluster of a is also in the same cluster of b. For example $a = (125)(37)(64) \subseteq b = (125)(3467)$.

I let $a \cup b$ denote the least upper bound of a and b with respect to this partial ordering and $a \cap b$ denote the greatest lower bound of a and b with respect to this partial ordering. I let 1 denote the unique 1-cluster partition and 0 denote the unique N cluster partition. For $a = (125)(37)(64)$ and $b = (125)(367)(4)$ these definitions imply $a \cap b = (125)(37)(4)(6)$, $a \cup b = (125)(3467)$, $1 = (1234567)$, and $0 = (1)(2)(3)(4)(5)(6)(7)$.

Next I introduce the operators that translate clusters. On each of the single-particle Hilbert-spaces, $\mathcal{H}_i$, there is a trivial representation of the three-dimensional Euclidean group

$$U_i(\mathbf{x}, R)|\mathbf{p}, \mu\rangle = \sum_{\mu'=-j}^{j} |R\mathbf{p}, \mu'\rangle e^{iR\mathbf{p}\cdot\mathbf{x}} D^j_{\mu'\mu}(R) \tag{3.3}$$

where $\mathbf{x}$ are parameters of the space translation subgroup and R is a rotation. The matrix $D^j_{\mu'\mu}(R)$ is the ordinary Wigner function. I define

$$U_a(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_a}, R_{n_a}) :=$$

$$\otimes_{i_1 \in a_1} U_{i_1}(\mathbf{x}_1, R_1) \otimes_{i_2 \in a_2} U_{i_2}(\mathbf{x}_2, R_2) \cdots \otimes_{i_{n_a} \in a_{n_a}} U_{i_{n_a}}(\mathbf{x}_{n_a}, R_{n_a}). \tag{3.4}$$

These operators perform independent translations and rotations on the subsystems of particles in each cluster of the partition a.

A bounded operator A on the N-particle Hilbert space has a cluster expansion if it can be expressed as a sum of terms associated with each partition a,

$$A = \sum_{a \in \mathcal{P}} [A]_a, \tag{3.5}$$

where the operators $[A]_a$ are invariant with respect to independent translations and rotations of the cluster of the partition a

$$[[A]_a, U_a(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_a}, R_{n_a})]_- = 0, \tag{3.6}$$

and vanish when any pair of particles in the same cluster of the partition a are asymptotically separated:

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \|[A]_a U_b(\mathbf{x}_1, R_1 \cdots, \mathbf{x}_{n_b}, R_{n_b}))|\psi\rangle\| = 0 \qquad b \not\supseteq a. \tag{3.7}$$

Equations (3.6 and 3.7) provide a mathematical characterization of these two properties. When A is unbounded I will assume that these equations hold for a suitable dense set of vectors $|\psi\rangle$.

For $b \supseteq a$, $U_b(\cdots)$ is a subgroup of $U_a(\cdots)$ so

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \|[A]_a U_b(\mathbf{x}_1, , R_1 \cdots, \mathbf{x}_{n_b}, R_{n_b})|\psi\rangle\| =$$

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \|U_b(\mathbf{x}_1, , R_1 \cdots, \mathbf{x}_{n_b}, R_{n_b})[A]_a|\psi\rangle\| = \|[A]_a|\psi\rangle\| \qquad b \not\supseteq a. \tag{3.8}$$

It follows from (3.6) and (3.7) that if A has a cluster expansion then

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \|(A - \sum_{b \supseteq a} [A]_a) U_a(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_b}, R_{n_b})|\psi\rangle\| = 0 \tag{3.9}$$

which leads to the definition

$$A_b := \sum_{b \supseteq a} [A]_a, \tag{3.10}$$

which is the part of A that is invariant with respect to translations of the individual clusters of b, irrespective of the asymptotic properties:

$$[A_b, U_b(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_b}, R_{n_b})]_- = 0. \tag{3.11}$$

This is the part of A that remains after the clusters of the partition b are asymptotically separated.

It is also useful to define

$$A^b := A - A_b = \sum_{b \not\supseteq a} [A]_a \tag{3.12}$$

which is the part of A that asymptotically vanishes when the different clusters of b are asymptotically separated:

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \| A^b U_b(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_b}, R_{n_b}) |\psi\rangle \| = 0. \tag{3.13}$$

The incidence matrix, $\delta_{a \supseteq b}$, called the zeta function of the partial ordering, $a \supseteq b$, has an inverse, called the Möbius function, $\delta^{-1}_{a \supseteq b}$ of the partial ordering, which also vanishes when $a \not\supseteq b$. The Möbius function can be used to express $[A]_a$ in terms of A_b:

$$[A]_a = \sum_{b \subseteq a} \delta^{-1}_{a \supseteq b} A_b. \tag{3.14}$$

This inverse is explicitly known [10]:

$$\delta^{-1}_{a \supseteq b} = \begin{cases} (-1)^{n_a} \prod_{i=1}^{n_a} (-)^{n_{b_i}} (n_{b_i} - 1)! & a \supseteq b \\ 0 & a \not\supseteq b \end{cases} \tag{3.15}$$

where n_{b_i} is the number of clusters of b contained in the ith cluster of a.

The following identities are consequences of the definitions

$$(AB)_a = A_a B_a \qquad (AB)^a = A_a B^a + A^a B_a + A^a B^a \qquad (A_a)_b = A_{a \cap b}. \tag{3.16}$$

If A has a cluster expansion the connected part of A is the part of A that vanishes when any pair of particles is separated. It is

$$[A]_1 = A - \sum_{a \neq 1} [A]_a. \tag{3.17}$$

Using properties of the Möbius and zeta functions gives the following expression for $[A]_1$:

$$[A]_1 = \sum_{a \in \mathcal{P}} \sum_{b \in \mathcal{P}} \delta^{-1}_{1 \supseteq a} \delta_{a \supseteq b} [A]_b = \sum_{a \in \mathcal{P}} \delta^{-1}_{1 \supseteq a} A_a = \delta^{-1}_{1 \supseteq 1} A_1 + \sum_{a \neq 1} \delta^{-1}_{1 \supseteq a} A_a = \tag{3.18}$$

$$A + \sum_{a \neq 1} \delta^{-1}_{1 \supseteq a} A_a \tag{3.19}$$

where I have used the identities

$$\delta^{-1}_{1 \supseteq 1} = 1 \qquad A_1 = A. \tag{3.20}$$

I define the coefficients

$$\mathcal{C}_a := -\delta^{-1}_{1 \supseteq a} = (-)^{n_a} (n_a - 1)! \tag{3.21}$$

from which it follows that

$$A = [A]_1 + \sum_{a \neq 1} \mathcal{C}_a A_a. \tag{3.22}$$

This separates the "connected" part $[A]_1$ of A from the disconnected part, $\sum_{a \neq 1} \mathcal{C}_a A_a$, of A.

IV. SCATTERING EQUIVALENCES

Of interest is a characterization of when two N-body Hamiltonians are physically equivalent. It is customary in the literature to call two Hamiltonians equivalent if they are related by a unitary transformation. This is really insufficient. For a simple counter example consider two different short-ranged repulsive two-body interactions, V_1 and V_2. The spectrum and multiplicity of the of the two-body Hamiltonians are identical. If the wave operators satisfy the completeness relations (2.17-2.18) then the operator

$$A = \Omega_+(H_1, \Phi, H_0)\Omega_+^\dagger(H_2, \Phi, H_0) \tag{4.1}$$

is a unitary operator on $\mathcal{H}$. It follows from the intertwining relations, (2.19), that A also satisfies $AH_2 = H_1A$; however any two arbitrary repulsive potentials do not give the same phase shifts. So even though H_1 and H_2 are related by a unitary transformation, the scattering observables are unrelated. For equivalent Hamiltonians I also need to require that the S matrix remains unchanged and the description of the free particles remains unchanged.

The two-Hilbert formulation of scattering is useful in this regard. What is required in general is the unitary equivalence of the Hamiltonians

$$H' = A^\dagger HA \qquad AA^\dagger = I \tag{4.2}$$

and S-matrix equivalence

$$S(H, \Phi, H_f) = S(H', \Phi', H_f), \tag{4.3}$$

where H_f remains unchanged. Recall from the construction of the previous section that the operator Φ also depends on H.

To determine the requirements of S-matrix equivalence on A I use (2.16) in (4.3) to obtain

$$\Omega_+^\dagger(H, \Phi, H_f)\Omega_-(H, \Phi, H_f) = \Omega_+^\dagger(H', \Phi', H_f)\Omega_-(H', \Phi', H_f). \tag{4.4}$$

Using (2.15) in (4.4) gives the following candidate for A:

$$A := \Omega_+(H, \Phi, H_f)\Omega_+^\dagger(H', \Phi', H_f) = \Omega_-(H, \Phi, H_f)\Omega_-^\dagger(H', \Phi', H_f). \tag{4.5}$$

The intertwining property (2.19) gives

$$AH' = HA. \tag{4.6}$$

Unitarity of A follows from (2.17-2.18), which also can be used to show

$$\Omega_+(H, \Phi, H_f) = \Omega_+(H, \Phi, H_f)I_{\mathcal{H}_f} =$$

$$\Omega_+(H, \Phi, H_f)\Omega_+^\dagger(H', \Phi', H_f)\Omega_+(H', \Phi', H_f) =$$

$$A\Omega_+(H',' \Phi, H_f) = \Omega_+(AH'A^\dagger, A\Phi', H_f) = \Omega_+(H, A\Phi', H_f). \tag{4.7}$$

Subtracting the left from the right side of (4.7) and using the definition of the wave operators gives the identity

$$0 = \Omega_+(H, \Phi, H_f) - \Omega_+(H, A\Phi', H_f) \tag{4.8}$$

which is equivalent to

$$0 = \lim_{t\to\infty} \|U(t)[\Phi - A\Phi']U_f(t)|\mathbf{f}\rangle\| = \lim_{t\to\infty} \|[\Phi - A\Phi']U_f(t)|\mathbf{f}\rangle\|. \tag{4.9}$$

Similarly using the second equation (4.4) gives the corresponding relation with the other time limit

$$0 = \lim_{t\to-\infty} \|[\Phi - A\Phi']U_f(t)|\mathbf{f}\rangle\|. \tag{4.10}$$

The vanishing of *both* time limits is important. The failure of S-matrix equivalence in the case of the two repulsive potentials is because the two time limits lead to *different* unitary operators, $A_+ \neq A_-$, satisfying (4.2).

The asymptotic conditions, (4.9-4.10), along with the definition of the operator A (4.5), are consequences of the identity (4.3) of the two scattering operators.

Conversely, if both asymptotic conditions, (4.9) and (4.10), hold for some unitary A then

$$\Omega_\pm(H,\Phi,H_f) = \Omega_\pm(H,A\Phi',H_f) = A\Omega_\pm(H',\Phi',H_f). \tag{4.11}$$

Because this holds for the same A for both time limits it follows that

$$S(H,\Phi,H_f) = \Omega_+^\dagger(H,\Phi,H_f)\Omega_-(H,\Phi,H_f) =$$

$$\Omega_+^\dagger(H',\Phi',H_f)A^\dagger A\Omega_-(H',\Phi',H_f) = S(H',\Phi',H_f). \tag{4.12}$$

This shows that the asymptotic conditions (4.9-4.10) are necessary and sufficient conditions for the invariance of the S-matrix. This result is the content of a theorem in formal scattering theory due to Ekstein [11].

I also need to determine the relation of Φ' to A and H in the context of Ekstein's theorem. I assume that A has a well-defined cluster expansion and I define an operator A_a by turning off the parts of A that vanish when the clusters of the partition a are asymptotically separated. It follows that if I turn off the interactions between particles in different clusters of the partition a that H' will have the following limiting form

$$H' = A^\dagger HA \to H'_a = A_a^\dagger H_a A_a \tag{4.13}$$

where H'_a is a sum of transformed subsystem Hamiltonians associated with each cluster. It follows from the definitions (2.7) and (2.9) that the channel injection operators Φ_{α_i} and Φ'_{α_i} associated with the partition a are related by

$$\Phi'_{\alpha_i} = A_a^\dagger \Phi_{\alpha_i} \tag{4.14}$$

where Φ'_{α_i} is an eigenstate of H'_a with eigenvalues

$$E_{\alpha_i} = \sum_{j=1}^{n_a}(\mathbf{p}_j^2/2m_j - \epsilon_j). \tag{4.15}$$

Thus

$$\Phi' = \sum_i A_{a_i}^\dagger \Phi_{\alpha_i}. \tag{4.16}$$

Finally, if I want the subsystem Hamiltonians to be separately rotationally and translationally invariant, then each of the operators A_a, obtained from A by turning off the parts of A that generate interactions between particles in different clusters of the partition a should also be translationally and rotationally invariant.

Given a unitary A with a cluster expansion, equations (4.14) and (4.16) imply

$$A\Phi' = \sum_i AA_{a_i}^\dagger \Phi_{\alpha_i}. \tag{4.17}$$

The requirement that H and $H' = A^\dagger HA$ give the same S matrix is that A is a unitary transformation with a well-defined cluster expansion satisfying the asymptotic conditions

$$0 = \lim_{t\to\pm\infty} \| \sum_i [I - AA_a^\dagger]\Phi_{\alpha_i} U_{\alpha_i}(t)|\mathbf{f}_{\alpha_i}\rangle\| = 0 \tag{4.18}$$

for each channel, or equivalently because of the unitarity of A

$$\lim_{t\to\pm\infty} \| \sum_i [A^\dagger - A_a^\dagger]\Phi_{\alpha_i} U_{\alpha_i}(t)|\mathbf{f}_{\alpha_i}\rangle\| = 0. \tag{4.19}$$

If I assume that all of the $\mathbf{f}_i$ vanish except for the N-body breakup channel then (4.18) implies

$$0 = \lim_{t\to\pm\infty} \| \sum_i [I - A^\dagger]U_0(t)|\mathbf{f}_0\rangle\| = 0. \tag{4.20}$$

When A has a suitable cluster expansion, (4.20) implies (4.18). This is discussed in section V.

Equation (4.20) is equivalent to

$$0 = \lim_{t\to\pm\infty} \| \sum_i [I - A]U_0(t)|\mathbf{f}_0\rangle\| = 0. \tag{4.21}$$

where we have used $\Phi_0 = I$ and $\mathcal{H}_0 = \mathcal{H}$ for the unique N-cluster breakup channel.

I refer to unitary transformations A satisfying (4.21) as scattering equivalences. It is easy to show that with this definition the set of scattering equivalences form a group with respect to operator multiplication.

V. ASYMPTOTIC PROPERTIES

It is now possible to construct a parameterized set of scattering equivalences. Because the scattering equivalences A are unitary operators, it follows that A can be expressed as the Cayley transform of a Hermitian operator Γ

$$A = \frac{1 - i\Gamma}{1 + i\Gamma} \qquad \Gamma = \Gamma^\dagger. \tag{5.1}$$

In what follows I will assume that the Cayley transform, Γ, has a cluster expansion,

$$\Gamma = \sum_{a \in \mathcal{P}} [\Gamma]_a \tag{5.2}$$

where the $[\Gamma]_a$ are Hermitian, invariant with respect to translations and rotations of the clusters of a, and vanish when any of the particles in different clusters of a are asymptotically separated. Specifically

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to \infty} \| [\Gamma]_a U_b(\mathbf{x}_1, R_1 \cdots, \mathbf{x}_{n_b}, R_{n_b}) |\psi\rangle \| = 0 \qquad b \not\supseteq a. \tag{5.3}$$

A sufficient condition to satisfy all of the cluster conditions is that $[\Gamma]_a$ and $T[\Gamma]_a T$, where T is the N-body kinetic energy operator, are both compact after one removes all of the momentum conserving delta functions. In what follows, rather than formally taking the cluster limit (5.3), I use a switching parameter to turn off the parts of the operators that vanish in the cluster limit. Thus, to take the limit where the clusters of a partition a are separated, I formally write

$$\Gamma(\lambda) = \Gamma_a + \lambda \Gamma^a \qquad \Gamma(1) = \Gamma \tag{5.4}$$

and take the limit that $\lambda \to 0$. I call this implementation of cluster properties algebraic clustering[12]; it separates the combinatorial aspects of cluster properties from the analytic aspects.

While the cluster expansions are based on asymptotic properties of the operators A with respect to translations, the limits of interest in this paper are the time limits (4.18-4.21). Although I will not get into the technical details of the cluster limits, it is important to understand the relation between the cluster limit and the time limit.

If I consider the time limit in equations (4.19), it has the form

$$\lim_{t \to \pm\infty} \| \sum_i [A^\dagger - A_a^\dagger] \Phi_{\alpha_i} U_{\alpha_i}(t) |\mathbf{f}_{\alpha_i}\rangle \| =$$

$$\lim_{t \to \pm\infty} \| \sum_i A^{a\dagger} e^{-i \sum (\frac{\mathbf{p}_{a_j}^2}{2m_{a_j}} - \epsilon_j) t} \Phi_{\alpha_i} |\mathbf{f}_{\alpha_i}\rangle \| = 0 \tag{5.5}$$

where the kinetic energy that appears in the exponent is the sum kinetic energies of each cluster of a. It looks similar to the cluster limit

$$\lim_{|\mathbf{x}_j - \mathbf{x}_k| \to \infty} \| \sum_i A^{a\dagger} e^{i \sum \mathbf{p}_{a_j} \cdot \mathbf{x}_j} \Phi_{\alpha_i} |\mathbf{f}_{\alpha_i}\rangle \| = 0. \tag{5.6}$$

To understand the relation between the limits in (5.5) and (5.6) I consider first a single degree of freedom. Consider the limit where the y-component of cluster i is being translated. The time limit above is bounded by a sum of terms of the form

$$\lim_{\lambda \to \infty} \int_{-\infty}^{+\infty} f(p_{iy}) e^{i p_{iy} \lambda} dp_{iy} =$$

$$\lim_{\lambda \to \infty} \int_0^\infty f(p_{iy}) e^{i p_{iy} \lambda} dp_{iy} + \lim_{\lambda \to -\infty} \int_0^\infty f(-p_{iy}) e^{i p_{iy} \lambda} dp_{iy}. \tag{5.7}$$

Both terms vanish by the Riemann Lebesgue lemma if $f(p_{iy})$ and $f(-p_{iy})$ are absolutely integrable on $[0, \infty]$.

The corresponding time limit (4.21) contains a term of the form

$$\lim_{\lambda \to \infty} \int_0^{+\infty} f(p_{iy}) e^{i \frac{p_{iy}^2}{2m_i} \lambda} dp_{iy}. \tag{5.8}$$

If I let $u = \frac{p_{iy}^2}{2m_i}$ the time limit becomes

$$\lim_{\lambda\to\infty}\int_{-\infty}^{\infty}(f(\sqrt{2m_iu})+f(-\sqrt{2m_iu}))e^{iu\lambda}\sqrt{\frac{m_i}{u}}du = \lim_{\lambda\to\infty}\int_0^{+\infty}g(u)e^{iu\lambda}du \tag{5.9}$$

where

$$g(u) := (f(\sqrt{2m_iu})+f(-\sqrt{2m_iu}))\sqrt{\frac{m_i}{u}} \tag{5.10}$$

is an absolutely integrable function of u if $f(p_{iy})$ is an absolutely integrable function p_{iy}. Using an extension of this same argument it is possible to show that the two limits (5.5) and (5.6) are equivalent, provided Φ_{α_i}, $\mathbf{f}_{\alpha_i}$ and A^a are all suitably well-behaved (i.e. so the resulting integrand is absolutely integrable).

This means that the time limit associated with a given channel has a vanishing limit whenever the space limit associated with the same channel also vanishes. Once I eliminate the delta functions, the compactness condition always ensures that (5.5) and (5.6) are satisfied. If the functions are smooth the fall-off is faster.

For channels associated with the partition a the operators A^a must vanish for both time limits. A sufficient condition for this to be satisfied for *all* partitions a is that

$$\lim_{t\to\pm\infty}\|(A-I)\Phi_0U_0(t)\Phi_0|\mathbf{f}_0\rangle\| = 0 \tag{5.11}$$

for the N cluster partition 0. In this case $\Phi_0 = I$, $\mathcal{H}_0 = \mathcal{H}$ and this condition becomes

$$\lim_{t\to\pm\infty}\|(A-I)U_0(t)\Phi_0|\mathbf{f}_0\rangle\| = 0 \tag{5.12}$$

This ensures that $I-A$ is a sum terms that vanish when all particles are asymptotically separated. This is the basis of our claim that (4.21) implies (4.19) and leads to the characterization (4.21) of the asymptotic properties of scattering equivalences.

VI. CONSTRUCTION

To construct a suitable class of operators A that can be used in variational calculations, consider operators A, where the Cayley transform has a cluster expansion

$$A = \frac{1-i\Gamma}{1+i\Gamma} \qquad \Gamma = \Gamma^\dagger. \qquad \Gamma = \sum_{a\in\mathcal{P}}[\Gamma]_a \tag{6.1}$$

where each $[\Gamma]_a$ is a Hermitian operator that commutes with $U_a(\mathbf{x}_1, R_1, \cdots, \mathbf{x}_{n_a}, R_{n_a})$ and satisfies the asymptotic condition

$$\lim_{|\mathbf{x}_i-\mathbf{x}_j|\to\infty}\|[\Gamma]_aU_b(\mathbf{x}_1,, R_1\cdots, \mathbf{x}_{n_b}, R_{n_b}))|\psi\rangle\| = 0 \qquad b\not\supseteq a. \tag{6.2}$$

I also assume that after the momentum conserving delta functions are removed, the remainder is a compact operator with respect to the internal variables. This ensures that (6.2) holds. The means that the internal part has an expansion of the form

$$[\Gamma]_a = I\times[\hat{\Gamma}]_a \tag{6.3}$$

where I is associated with the delta functions and compact remainder has the canonical form

$$[\hat{\Gamma}]_a = \sum_n|\xi_{an}\rangle\lambda_{an}\langle\xi_{an}| \tag{6.4}$$

with $\lambda_{an} = \lambda_{an}^*$, $\lim_{n\to\infty}|\lambda_{an}|\to 0$ and $\langle\xi_{am}|\xi_{an}\rangle = \delta_{mn}$. In a variational framework the coefficients λ_{an} and the orthogonal vectors $|\xi_{an}\rangle$ can be chosen to depend on variational parameters.

In general the operators $[\hat{\Gamma}]_a$, along with the original Hamiltonian, are the input to any calculation. In addition, because of Ekstein's theorem, the transformation leads to scattering equivalent Hamiltonian characterized by a scattering equivalence with a cluster expansion of the form (3.5). The Cayley transform may be unbounded, but it will have and algebraic cluster expansion of the above form.

The cluster expansion of Γ can be used to generate the cluster expansion of A. Since Γ_a and $[\Gamma]_a$ are related by the Möbius and zeta functions, it is possible to construct Γ_a from the $[\Gamma]_b$'s.

I have

$$\Gamma_a = \sum_b \delta_{a \supseteq b} [\Gamma]_b \tag{6.5}$$

$$A_a = \frac{1 - i\Gamma_a}{1 + i\Gamma_a} \tag{6.6}$$

$$[A]_a = \sum \delta^{-1}_{a \supseteq b} A_b. \tag{6.7}$$

The A_a's can be computed recursively on the number of clusters in the partition, starting with $N-1$ cluster partitions.

The nature of the general construction can be illustrated using a three-body example. In this case $\Gamma_{(ij)(k)} = [\Gamma]_{(ij)(k)}$. For the two cluster partitions, $a = (ij)(k)$, I first solve the integral equation

$$\frac{1}{i - \Gamma_{(ij)(k)}} = \frac{1}{i} - i[\Gamma]_{(ij)(k)} \frac{1}{i - \Gamma_{(ij)(k)}}. \tag{6.8}$$

For finite rank $[\Gamma]_{(ij)(k)}$ this is an algebraic problem. $[\Gamma]_a$'s of the form (6.4) can be uniformly approximated by finite rank $[\Gamma]_a$. For the special case that $[\Gamma]_a = \lambda \Pi_a$ is a real constant multiplied by the direct product of the identity (in the conserved momentum variables) and a rank-one projection operator, equation (6.8) can be solved analytically. The solution is

$$A_{(ij)(k)} = \frac{1 - i[\Gamma]_{(ij)(k)}}{1 + i[\Gamma]_{(ij)(k)}} = I - \frac{2i\lambda}{1 + i\lambda} \Pi_{(ij)(k)}. \tag{6.9}$$

To use these solutions to compute A I define

$$R := \frac{1}{1 + i\Gamma} \tag{6.10}$$

$$R_{(ij)(k)} = \frac{1}{I + i[\Gamma]_{(ij)(k)}} \tag{6.11}$$

and

$$R_{(1)(2)(3)} = I. \tag{6.12}$$

For the special case of a rank one $\Gamma_{(ij)(k)}$

$$R_{(ij)(k)} = I - i \frac{\lambda_{(ij)(k)}}{1 + i\lambda_{(ij)(k)}} \Pi_{(ij)(k)}. \tag{6.13}$$

In general the operators $R_{(ij)(k)}$ and R satisfy the resolvent identities

$$R_{(ij)(k)} = I - i[\Gamma]_{(ij)(k)} R_{(ij)(k)} \tag{6.14}$$

and

$$R = R_{(ij)(k)} - iR_{(ij)(k)}([\Gamma]_{(jk)(i)} + [\Gamma]_{(ki)(j)} + [\Gamma]_{(123)})R \tag{6.15}$$

$$R = R_{(1)(2)(3)} + i\Gamma R \tag{6.16}$$

To get an equation for R note that (3.15) and (3.21) imply

$$\sum_{a \neq 1} \mathcal{C}_a = 1. \tag{6.17}$$

Using this with equations (3.21) gives the following equation for R:

$$R = \sum_{a\neq 1} \mathcal{C}_a R = \sum_{a\neq 1} \mathcal{C}_a R_a - i \sum_{a\neq 1} \mathcal{C}_a R_a \Gamma^a R. \tag{6.18}$$

Equation (6.18) is valid for any number of particles. For the three-particle case the driving term and kernel of (6.18) can be expressed in terms of the $[\Gamma]_a$ as

$$\sum_{a\neq 1} \mathcal{C}_a R_a = R_{(ij)(k)} + R_{(ij)(k)} + R_{(ij)(k)} - 2I =$$

$$I - i[\Gamma]_{(12)(3)} R_{(12)(3)} - i[\Gamma]_{(23)(1)} R_{(23)(1)} - i[\Gamma]_{(31)(2)} R_{(31)(2)} \tag{6.19}$$

and

$$-i \sum_{a\neq 1} \mathcal{C}_a R_a \Gamma^a =$$

$$-i(I - i[\Gamma]_{(12)(3)} R_{(12)(3)})([\Gamma]_{(23)(1)} + [\Gamma]_{(31)(2)} + [\Gamma]_{(123)})$$

$$-i(I - i[\Gamma]_{(23)(1)} R_{(23)(1)})([\Gamma]_{(31)(2)} + [\Gamma]_{(12)(3)} + [\Gamma]_{(123)})$$

$$-i(I - i[\Gamma]_{(31)(2)} R_{(31)(2)})([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)} + [\Gamma]_{(123)})$$

$$+i2I([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)}[\Gamma]_{(31)(2)} + [\Gamma]_{(123)}) \tag{6.20}$$

$$= -i[\Gamma]_{(123)} - [\Gamma]_{(12)(3)} R_{(12)(3)}([\Gamma]_{(23)(1)} + [\Gamma]_{(31)(2)} + [\Gamma]_{(123)})$$

$$-[\Gamma]_{(23)(1)} R_{(23)(1)}([\Gamma]_{(31)(2)} + [\Gamma]_{(12)(3)} + [\Gamma]_{(123)})$$

$$-[\Gamma]_{(31)(2)} R_{(31)(2)}([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)} + [\Gamma]_{(123)}). \tag{6.21}$$

The important observation is that this operator, which is the kernel of the integral equation (6.18), is compact after delta functions that arise from overall translational invariance are removed. It follows that equation (6.18) can be solved my standard Fredholm methods. The solution can then be used to construct A using

$$A = \frac{1 - i\Gamma}{1 + i\Gamma} = (1 - i\Gamma)R = \tag{6.22}$$

$$(I - i([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)} + [\Gamma]_{(31)(2)} + [\Gamma]_{(123)})R. \tag{6.23}$$

If the individual $[\Gamma]_a$ are finite rank (after all of the delta functions due to the translational symmetry are removed) then it follows that the kernel (6.21) is finite rank (after the overall momentum conserving delta function is removed) . This is most easily seen in the special case where all of the $[\Gamma]_a$ are proportional to one-dimensional projectors (after the delta functions are removed). In this case the kernel (6.21) becomes

$$-i\lambda_{(123)}\Pi_{(123)} - \frac{\lambda_{(12)(3)}}{1 + i\lambda_{(12)(3)}}\Pi_{(12)(3)})(\lambda_{(23)(1)}\Pi_{(23)(1)} + \lambda_{(31)(2)}\Pi_{(31)(2)}\lambda_{(123)}\Pi_{(123)}$$

$$-\frac{\lambda_{(23)(1)}}{1 + i\lambda_{(23)(1)}}\Pi_{(23)(1)})(\lambda_{(31)(2)}\Pi_{(31)(2)} + \lambda_{(12)(3)}\Pi_{(12)(3)}\lambda_{(123)}\Pi_{(123)}$$

$$-\frac{\lambda_{(31)(2)}}{1+i\lambda_{(31)(2)}}\Pi_{(31)(2)})(\lambda_{(12)(3)}\Pi_{(12)(3)}+\lambda_{(23)(1)}\Pi_{(23)(1)}\lambda_{(123)}\Pi_{(123)}. \tag{6.24}$$

This is a finite dimensional matrix involving the ten operators $\Pi_{(123)}$, $\Pi_{(12)(3)}\Pi_{(23)(1)}$, $\Pi_{(12)(3)}\Pi_{(31)(2)}$, $\Pi_{(12)(3)}\Pi_{(123)}$, $\Pi_{(23)(1)}\Pi_{(31)(2)}$, $\Pi_{(23)(1)}\Pi_{(12)(3)}$, $\Pi_{(23)(1)}\Pi_{(123)}$, $\Pi_{(31)(2)}\Pi_{(23)(1)}$, $\Pi_{(31)(2)}\Pi_{(12)(3)}$, and $\Pi_{(31)(2)}\Pi_{(123)}$. After the overall momentum conserving delta function is removed the range of the this operator is a ten dimensional vector space. The resulting integral equation involves solving a system of 10 linear equations. When the operators $[\Gamma]_a$ are finite rank, rather than rank one, the matrix is larger, but it is still finite dimensional.

This construction can be extended to any number of particles. The kernel of the integral equation for the N-body R is still finite rank if all of the input $[\Gamma]_a$ are finite rank. Thus, for finite rank $[\Gamma]_a$ the construction of A involves only quadratures and linear algebra.

Returning to the three-body example have

$$H = T + V_{(12)(3)} + V_{(23)(1)} + V_{(31)(2)} + V_{(123)} \tag{6.25}$$

$$A_{(1)(2)(3)} = I \tag{6.26}$$

$$[A]_{(12)(3)} = (I - i[\Gamma]_{(12)(3)})R_{(12)(3)} - I = -2i[\Gamma]_{(12)(3)}R_{(12)(3)} \tag{6.27}$$

$$[A]_{(23)(1)} = (I - i[\Gamma]_{(23)(1)})R_{(23)(1)} - I = -2i[\Gamma]_{(23)(1)}R_{(23)(1)} \tag{6.28}$$

$$[A]_{(31)(2)} = (I - i[\Gamma]_{(31)(2)})R_{(31)(2)} - I = -2i[\Gamma]_{(31)(2)}R_{(31)(2)} \tag{6.29}$$

$$[A]_{(123)} = -i\sum_{a\neq 1}\mathcal{C}_a R_a \Gamma^a R = \tag{6.30}$$

$$R_{(12)(3)}([\Gamma]_{(23)(1)} + [\Gamma]_{(31)(2)} + [\Gamma]_{(123)})R+$$

$$R_{(23)(1)}([\Gamma]_{(31)(2)} + [\Gamma]_{(12)(3)} + [\Gamma]_{(123)})R+$$

$$R_{(31)(2)}([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)} + [\Gamma]_{(123)})R$$

$$-2([\Gamma]_{(12)(3)} + [\Gamma]_{(23)(1)} + [\Gamma]_{(31)(2)} + [\Gamma]_{(123)})R \tag{6.31}$$

I can use these cluster expansions of the scattering equivalences to determine the cluster expansion of the transformed three-body Hamiltonian

$$H' = A^\dagger H A \tag{6.32}$$

$$H'_a = A_a^\dagger H_a A_a \tag{6.33}$$

$$[H']_1 = H' - \sum_{a\neq 1}\mathcal{C}_a H'_a = A^\dagger H A - \sum_{a\neq 1}\mathcal{C}_a A_a^\dagger H_a A_a. \tag{6.34}$$

This means that the transformed two-body interactions are

$$V'_{(ij)(k)} = [H']_{(ij)(k)} = (I + [A]^\dagger_{(ij)(j)})(T + V_{(ij)(k)})(I + [A]_{(ij)(j)}) - T = \tag{6.35}$$

$$V_{(ij)(k)} + [A]^\dagger_{(ij)(j)}V_{(ij)(k)} + [A]^\dagger_{(ij)(j)}T + [A]^\dagger_{(ij)(j)}T[A]_{(ij)(j)}+$$

$$[A]^\dagger_{(ij)(j)})V_{(ij)(k)}[A]_{(ij)(j)} + V_{(ij)(k)}[A]_{(ij)(j)} + T[A]_{(ij)(j)} \tag{6.36}$$

where T is the three-body kinetic energy and the $A_{(ij)(k)}$ are given by (6.27-6.29).

An important observation is that $V'_{(ij)(k)}$ only depends on T, $V_{(ij)(k)}$, and $[\Gamma]_{(ij)(k)}$. It does not depend on $[\Gamma]_{(123)}$. This means that after one chooses $[\Gamma]_{(ij)(k)}$ to give a transformed two-body interaction, it is still possible to use the freedom to *independently* choose $[\Gamma]_{(123)}$ to transform the resulting three-body interaction without changing the transformed two-body interactions.

The transformed three-body interaction is

$$V'_{(123)'} = A^\dagger HA - T - V'_{(12)(3)} - V'_{(23)(1)} - V'_{(31)(2)} = [A^\dagger HA]_1 = \tag{6.37}$$

$$[A]_{(123)}HA^\dagger +$$

$$[A]_{(12)(3)}\Big((T+V_{(12)(3)})([A]^\dagger_{(23)(1)} + [A]^\dagger_{(31)(2)} + [A]^\dagger_{(123)}) + (V_{(23)(1)} + V_{(31)(2)} + V_{(123)})A^\dagger\Big) +$$

$$[A]_{(23)(1)}\Big((T+V_{(23)(1)})([A]^\dagger_{(31)(2)} + [A]^\dagger_{(12)(3)} + [A]^\dagger_{(123)}) + (V_{(31)(2)} + V_{(12)(3)} + V_{(123)})A^\dagger\Big) +$$

$$[A]_{(31)(2)}\Big((T+V_{(31)(2)})([A]^\dagger_{(12)(3)} + [A]^\dagger_{(23)(1)} + [A]^\dagger_{(123)}) + (V_{(12)(3)} + V_{(23)(1)} + V_{(123)})A^\dagger\Big) +$$

$$T[A]^\dagger_{(123)} + V_{(12)(3)}([A]^\dagger_{(23)(1)} + [A]^\dagger_{(31)(2)} + [A]^\dagger_{(123)}) +$$

$$V_{(23)(1)}([A]^\dagger_{(31)(2)} + [A]^\dagger_{(12)(3)} + [A]^\dagger_{(123)}) +$$

$$V_{(31)(2)}([A]^\dagger_{(12)(3)} + [A]^\dagger_{(23)(1)} + [A]^\dagger_{(123)}). \tag{6.38}$$

This is expressed as a sum of completely connected terms; it could be expressed in a more symmetric form but that would involve more terms. The entire expression depends on the operators $[\Gamma]_a$ that depend on the variational parameters.

If the $[A]_{(1j)(k)}$ have already been determined by fixing the two-body interaction then one can start with the transformed potential and use an A where only $[\Gamma]_{(123)]}$ is non-zero to get an optimized three-body interaction. Alternatively one could state with the original potential and leave the $[A]_{(ij)(k)}$ fixed in the above expression, with all of the variational parameters in $[\Gamma]_{(123)}$.

VII. CONTROLLING THE HAMILTONIAN

I order to use variational methods to determine the best choice of Hamiltonian a positive functional is needed that can be minimized. It is possible to either work recursively on the number of particles, by first determining two-body interactions, followed by the three-body interaction, or alternatively to determine all interactions simultaneously.

The simplest type of functionals are of the form

$$F(V) = \mathrm{Tr}(\rho V^\dagger V)^{1/2} \tag{7.1}$$

where ρ is a positive, rotationally and translationally invariant operator. The trace is only taken over the variables that remain *after* the momentum conserving delta functions are removed. Thus for two-body interactions of the form

$$V(\mathbf{k}, \mathbf{k}', \eta_1 \cdots \eta_N)\delta(\mathbf{p}' - \mathbf{p}) \tag{7.2}$$

$F(V)$ would have the general form

$$F(V) = \int d\mathbf{k}d\mathbf{k}'d\mathbf{k}''V(\mathbf{k}, \mathbf{k}', \eta_1 \cdots \eta_N)V^*(\mathbf{k}'', \mathbf{k}', \eta_1 \cdots \eta_N)\rho(\mathbf{k}, \mathbf{k}'') \tag{7.3}$$

with obvious generalizations for three-body interaction.

$$F(V) = \int d\mathbf{k}d\mathbf{k}'d\mathbf{k}''V(\mathbf{k}-\mathbf{k}',\eta_1\cdots\eta_N)V^*(\mathbf{k}'-\mathbf{k}'',\eta_1\cdots\eta_N)\rho(\mathbf{k}''-\mathbf{k}') \tag{7.4}$$

If the starting potential is local this expression has to be modified because $VV^\dagger$ is a function of the difference $\mathbf{k}'-\mathbf{k}$ which leads to an infinite volume factor. While local potentials can be treated by using a different positive functional, an alternative is to note that if $V = V_{loc} + V_r$ then $F(V) = F(V_{loc}) + F'(V_r, V_{loc})$. It is only the first term that is infinite, but this term does not depend on the variational parameters. The second term will be finite for suitable A and it contains all of the dependence on the variational parameters. It follows that the critical value of the variational parameters can be determined by requiring that all partial derivatives of the second term at the critical value of the parameters.

The general procedure is to start from a given N-body Hamiltonian, H, and a parameterized set of scattering equivalences $A(\eta_1,\cdots,\eta_n)$ where η_i are variational parameters. The scattering equivalences $A(\eta_1,\cdots,\eta_n)$ generate a parameterized set of equivalent Hamiltonians:

$$H'(\eta_1,\cdots,\eta_n) = A^\dagger(\eta_1,\cdots,\eta_n)HA(\eta_1,\cdots,\eta_n). \tag{7.5}$$

They have cluster expansions

$$H' = T + \sum_{ij} V'_{ij}(\eta_1,\cdots,\eta_n) + \sum_{ijk} V'_{ijk}(\eta_1,\cdots,\eta_n) + \cdots + V'_N(\eta_1,\cdots,\eta_n). \tag{7.6}$$

The two, three, four $\cdots$ N-body interactions all depend on the choice of variational parameters.

For example, to construct two-body interactions that have primarily low-momentum content I would choose a functional that is large when the momenta are large. The functional has to be chosen so the trace is finite for all interactions in the model space.

A functional of the form

$$\rho(\mathbf{k},\mathbf{k}') = \tanh(\alpha + \mathbf{k}^2/\mathbf{k}_0^2)\tanh(\alpha + \mathbf{k}'^2/\mathbf{k}_0^2), \tag{7.7}$$

where α is a small dimensionless quantity, would suppress momentum components above the scale $\mathbf{k}_0^2$. Alternatively I can design positive functionals that weaken three-body forces or reduce two-body correlations.

Finding minimum of the functional

$$\mathrm{Tr}(\rho V_{12}^\dagger(\eta_1,\cdots,\eta_n)V_{12}(\eta_1,\cdots,\eta_n)) \tag{7.8}$$

with respect to the parameters $\eta_1,\cdots,\eta_n$ selects equivalent potentials that have low-momentum content.

After the two, three, $\cdots N-$body interactions have been determined, then I can use the new Hamiltonian as the starting point. I can construct a new set of interactions using scattering equivalences with $[\Gamma]_{(ij)(k)} = 0$. These scattering equivalences only affect the three and more-body interactions. I can choose a new three-body ρ that emphasizes some desirable feature of the three-body interaction. The local minimum generates a new three-body interaction. Combining the two scattering equivalences leads to an scattering equivalence A that transforms $H'' = A^\dagger HA$.

If this is embedded in the N-particle Hilbert space it (1) generates the selected two and three-body interactions, (2) new $4, 5\cdots N$-body interactions, and (3) explicit unitary transformations, A, that can be used to generate transformed operators like electromagnetic current operators

$$J^{\mu'}(x) = A^\dagger J^\mu(x)A. \tag{7.9}$$

VIII. SIMPLE EXAMPLE

To illustrate the method I consider a two-body Hamiltonian of the form

$$H = \frac{\mathbf{k}^2}{2\mu} + V, \tag{8.1}$$

where I assume that V is a local potential. I consider a parameterized rank one unitary transformation of the form

$$A(\lambda) = I + |g\rangle\frac{2i\lambda}{1 - i\lambda\langle g|g\rangle}\langle g| = I + |g\rangle f(\lambda)\langle g| \tag{8.2}$$

where $|g\rangle$ is a fixed form factor and λ is a variational parameter. The transformed potential is

$$V'(\lambda) = A^\dagger(\lambda) H A(\lambda) - \frac{\mathbf{k}^2}{2\mu}. \tag{8.3}$$

The transformed potential differs from the original potential by the addition of a finite number of separable terms. It has the form

$$V'(\lambda) = V + |g\rangle f^*(\lambda)\langle g|H + H|g\rangle f(\lambda)\langle g| + |g\rangle f^*(\lambda)\langle g|H|g\rangle f(\lambda)\langle g| = V + V_r(\lambda) \tag{8.4}$$

The first term in this expression is local but independent of λ. The remaining terms are separable and depend on λ.

I use the density (7.7), with a chosen value of $\mathbf{k}_0$. It has the form

$$\rho = |\chi\rangle\langle\chi| \tag{8.5}$$

leads to the variational function

$$F(\lambda) := \langle\chi| \left(V^{\dagger\prime}(\lambda)V'(\lambda) - V^\dagger V\right)|\chi\rangle = \langle\chi| \left(V^\dagger V_r(\lambda) + V_r^\dagger(\lambda)V + V_r^\dagger(\lambda)V_r(\lambda)\right)|\chi\rangle. \tag{8.6}$$

The subtracted contribution, $V^\dagger V$, eliminates the infinite constant that appears for local V. The terms in the resulting expression are

$$F(\lambda) =$$

$$\langle\chi|V^\dagger|g\rangle f^*(\lambda)\langle g|H|\chi\rangle + \langle\chi|V^\dagger H|g\rangle f(\lambda)\langle g|\chi\rangle + \langle\chi|V^\dagger|g\rangle f^*(\lambda)\langle g|H|g\rangle f(\lambda)\langle g|\chi\rangle +$$

$$\langle\chi|g\rangle f^*(\lambda)\langle g|HV|\chi\rangle + \langle\chi|H|g\rangle f(\lambda)\langle g|V|\chi\rangle + \langle\chi|g\rangle f^*(\lambda)\langle g|H|g\rangle f(\lambda)\langle g|V|\chi\rangle +$$

$$(\langle\chi|g\rangle f^*(\lambda)\langle g|H + \langle\chi|H|g\rangle f(\lambda)\langle g| + \langle\chi|g\rangle f^*(\lambda)\langle g|H|g\rangle f(\lambda)\langle g|) \times$$

$$(|g\rangle f^*(\lambda)\langle g|H|\chi\rangle + H|g\rangle f(\lambda)\langle g|\chi\rangle + |g\rangle f^*(\lambda)\langle g|H|g\rangle f(\lambda)\langle g|\chi\rangle). \tag{8.7}$$

This has the form

$$F(\lambda) = c_1 f(\lambda) + c_1^* f^*(\lambda) + c_2 f(\lambda) f^*(\lambda) + c_3 f^2(\lambda) f^*(\lambda) + c_3^* f^{*2}(\lambda) f(\lambda) + c_4 (f(\lambda) f^*(\lambda))^2 \tag{8.8}$$

with

$$f(\lambda) = \frac{2i\lambda}{1 - i\lambda\langle g|g\rangle}. \tag{8.9}$$

The coefficients c_k are liner combinations of the integrals $\langle\chi|V^\dagger|g\rangle$, $\langle g|H|\chi\rangle$, $\langle\chi|V^\dagger H|g\rangle$, $\langle g|HV|\chi\rangle$, $\langle g|\chi\rangle$, $\langle g|H|g\rangle$, $\langle g|g\rangle$ and $\langle g|H^2|g\rangle$. Since these do not involve λ they only have to be computed once. Although $f(\lambda)$ is complex, $F(\lambda)$ is a real function of λ. The λ dependence is a rational function.

The critical value of $\lambda = \lambda_c$ is determined by solving $\frac{dF}{d\lambda}(\lambda_c) = 0$ for λ_c. The resulting transformed Hamiltonian

$$H' = \frac{\mathbf{k}^2}{2\mu} + V'(\lambda_c) \tag{8.10}$$

gives the same binding energies and phase shifts as the original potential of any value of λ. The critical value of λ will lead to a potential that suppress momenta above $\mathbf{k}_0^2$. Obviously a softer potential will result if a larger class of unitary transformations A are used.

The original Hamiltonian did not have to be diagonalized to find the new potential. In this case, by varying λ from 0 to its critical value it is possible to continuously evolve the initial local potential to the final soft potential.

Since the unitary scattering equivalence is given as an explicit operator valued function of λ, I can calculate how observables evolve with the parameter λ. For example the electromagnetic current operators transforms as follows:

$$J^\mu(x)' = J^\mu(x) + f^*(\lambda)|g\rangle\langle g|J^\mu(x) + f(\lambda)J^\mu(x)|g\rangle\langle g| + f^*(\lambda)f(\lambda)|g\rangle\langle g|J^\mu(x)|g\rangle\langle g| \tag{8.11}$$

Finally, give the two-body unitary transformation for each pair of particles, $A_{ij}(\lambda)$, it is possible to construct the corresponding three-body unitary operator following the method of the previous section. In terms of the above parameters, for three identical particles A has the form

$$A = \frac{I - i\alpha}{I + i\alpha} \tag{8.12}$$

with

$$\alpha = i\frac{f(\lambda)}{2 + f(\lambda)\langle g|g\rangle}\left(|g_{12}\rangle\langle g_{12}| + |g_{23}\rangle\langle g_{23}| + |g_{31}\rangle\langle g_{31}|\right). \tag{8.13}$$

If the symmetric product of this unitary transformation for each pair is applied to the corresponding three-body Hamiltonian the transformed three-body Hamiltonian will have the form

$$H' = A^{\dagger}(\lambda)HA = K + V'_{12}(\lambda) + V'_{23}(\lambda) + V'_{31}(\lambda) + V'_{123}(\lambda). \tag{8.14}$$

The three-body force terms will appear even if the original Hamiltonian has only two-body forces. The computation of A from (8.12) involves quadratures and linear algebra, as discussed in section VI.

The evolution of the current and the three-body Hamiltonian from their original to their final values can be determined by varying λ from zero to the critical value, λ_0.

IX. CONCLUSION

In this paper I determined conditions that are necessary and sufficient for two Hamiltonains to be physically equivalent. I used the characterization of these unitary operators to construct a large class of equivalent N-body Hamiltonians that depend on variational parameters. There is considerable freedom in choosing the space of equivalent Hamiltonians. By choosing functions whose local minima select Hamiltonians with desirable properties from the space of equivalent Hamiltonians, it is possible to select classes of equivalent potentials with desirable properties. The general freedom available allows for the possibility of selecting two-body interactions with desirable properties, then subsequently selecting among equivalent three-body interactions with desirable properties. This procedure can be continued for any number of particles, allowing independent control of the two, three, four, $\cdots$ interactions. Because the k-body parts of A affect all operators with k or more particles, one hopes that desirable properties of the k-body interaction might persist for the $k + m$ body problems.

While in general it is possible to systematically weaken three and more-body interactions using these methods, it is not generally possible to eliminate them. The extremal interactions that are generated are not fundamental, they depend specifically on the choice of positive functional that is used to select these interactions.

The selection of equivalent potentials does not require diagonalizing any Hamiltonians; it only requires finding local minima of some user defined functionals. The functionals are designed so they get large for interactions with undesirable features. Once the operators $[\Gamma]_a$ are determined variationally, it is then possible to construct scattering equivalences A that operate on systems of any number of particles, and can be used to construct equivalent observables in the transformed representation. For a large class of variational Hamiltonians the operators A can be constructed from the Γ_a by finite linear algebra.

The general method can be combined with other methods, such are renormalization group methods, to reduce the strength of the transformed three-body force without changing the transformed two-body interactions.

The characterization of the group of scattering equivalences demonstrates the large class of equivalent Hamiltonains that can be selected by considering only spectral properties and scattering observables. This leads to a lot of flexibility in building equivalent models of the quantum N-body problem.

The author would like to acknowledge support for this work by the U. S. Department of Energy, Office of Nuclear Physics, under contract No. DE-FG02-86ER40286.

[1] S. Okubo, Prog. Theor. Phys. **12**, 603 (1954).
[2] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
[3] S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rept. **386**, 1 (2003), nucl-th/0305035.
[4] A. Nogga, S. K. Bogner, and A. Schwenk, Phys. Rev. **C70**, 061002(R) (2004), nucl-th/0405016.
[5] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. **C75**, 061001(R) (2007), nucl-th/0611045.

[6] E. Epelbaum, W. Glöckle, and U.-G. Meissner, Nucl. Phys. **A671**, 295 (2000), nucl-th/9910064.
[7] W. Glöckle and W. N. Polyzou, Few-Body Systems **9**, 97 (1990).
[8] Joseph P. S. King, ed., *Gian-Carlo Rota on Combinatorics* (Birkhauser, 1995).
[9] W. N. Polyzou, J. Math. Phys. **21**, 506 (1980).
[10] K. L. Kowalski, W. N. Polyzou, and E. F. Redish, J. Math. Phys. **22**, 1965 (1981).
[11] H. Ekstein, Phys. Rev. **117**, 1590 (1960).
[12] F. Coester and W. N. Polyzou, Phys. Rev. **D26**, 1348 (1982).