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Analytic methods for refined resonating group calculations[1]) 1: Reduction to cluster modes

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Abstract. The method of integral transforms is used to obtain the resonating group kernels for antisymmetrized n-nucleon problems. The result is given analytically for an arbitrary number of clusters and the so-called oscillator restriction of equal width parameters for all clusters is overcome. The analytic result is obtained by taking advantage of generating function properties of the integral transform used and is conveniently expressed in terms of DC-symbols that characterize the essential permutations from the antisymmetrizer.

1. Introduction

The treatment of nuclear systems by resonating group techniques [1, 2, 3, 4, 5] has made great progress in recent years. Remarkable results were achieved ranging from very detailed studies of reactions in small systems including many open channels, polarizations and sequential decays [6] to high spin states in certain heavy ion reactions [5, 7]. To achieve these results the techniques were considerably improved [3, 4, 5].

The technical question may roughly be separated in three parts: first there is the problem of antisymmetrization, present in any n-fermion system. This point has been discussed extensively in the literature and we shall take advantage of recent formulations in terms of double cosets [8]. Second there is the analytic problem of obtaining the resonating group kernels, subject of the present paper. Finally there is the problem of solving the coupled integro-differential equations, which is quite serious if many open channels are considered. An effective technique is provided by a generalization of Kohn's method [4].

Setting up the kernels implies integrating over the internal coordinates of the clusters. The approximation of the coupled integro-differential equations by linear equations, e.g., according to [4] implies integrating over the relative motion modes of

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[2]) This work was essentially finished at the time of the unfortunate death of our friend and teacher H. H. Hackenbroich T.H.S.; W.Z.

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the clusters. If more than two clusters are considered this presents quite serious analytical problems that will be treated in the second paper of this series.

In this paper we shall give an analytic expression for the integral kernels that may occur if a wave function with κ clusters is proposed. We will use integral transforms following early ideas of Hill and Wheeler [9]. This is possible because of recently developed methods [10, 11, 12] that allow for overcoming the so-called oscillator limitation. We shall discuss this point extensively and outline a scheme that may be applied for quite a general class of Gaussian integral transforms. Also we shall introduce a particular transform and implement this scheme.

For this purpose we choose the H-transform because we wish to give the most recent version of the analytical methods applied in the 'refined cluster model' program chain to computations in nuclear systems with $3 \leq A \leq 12$ [6, 13, 14]. In the derivation of the results we shall make any specializations as late as possible in order that the generality of the method is put to evidence.

The cluster wave functions [3], used for resonating group calculations, may be written as a superposition of functions of the form

$$\Psi = \mathscr{A}\left(\prod_{i=1}^{\kappa} \varphi_i\right)\chi\Xi. \tag{1.1}$$

Here $\mathscr{A}$ is the antisymmetrizer, φ_i the internal wave function of the ith cluster depending on the relative vectors of its n_i nucleons, χ the relative motion function of the clusters and Ξ an n-nucleon spin-isospin function. The functions φ_i must be square integrable and will be chosen as oscillator functions of arbitrary independent width while the functions χ need not necessarily vanish asymtotically in all of the relative motion variables $\vec{R}^1 \cdots \vec{R}^{\kappa-1}$ of the clusters since we wish to describe reactions.

For each term of the superposition we can and often will assume different channel spins, isospins, supermultiplets, as well as cluster structures, orbital angular momenta and other orbital characteristics of the wave functions. The superposition is only required to have good total angular momentum and parity. This allows for a quite general class of wave functions.

If we are interested in the action of any operator Op on the relative motion modes χ we shall have to integrate its action over the internal functions φ_i to obtain the kernel of the corresponding integral operator acting on χ.

As we shall also have to consider couplings between the different terms of the superposition the most general term in the kernel can be written symbolically

$$\mathscr{K}(\bar{\vec{\mathbf{R}}}, \vec{\mathbf{R}}) = \left\{\int \prod_{i=1}^{\bar{\kappa}} \bar{\varphi}_i \bar{P}\ \mathrm{Op}\ P \prod_{i=1}^{\kappa} \varphi_i\right\} \delta(\bar{\vec{R}}^{\bar{\kappa}}, \vec{R}^{\kappa}). \tag{1.2}$$

Here and in what follows the barred $(-)$ quantities always indicate quantities similar to the unbarred ones for another term of the superposition. P is a permutation from the antisymmetrizer and $\vec{R}^{\kappa}$ indicates the c.m. vector which we included with a reproducing kernel (Dirac δ) for later convenience. $\vec{\mathbf{R}}$ stands for a 3κ-dimensional vector with components $R_1^1, R_2^1, R_3^1; R_1^2, \ldots, R_3^{\kappa}$.

The expression for the kernel is symbolical because the integral might yield further Dirac δ's and it would have to be written very carefully for each set of permutations $\bar{P}$, P if variables were to appear explicitly. If the functions φ_i are oscillator functions of arbitrary width and the operator is made up of Gaussians, powers and derivatives, the integral can be performed [3] but direct evaluation is practical only for the lightest nuclear systems.

As mentioned before the use of integral transforms simplifies this task considerably. In the next section we shall proceed to discuss a particular transform, the H-transform, and we shall derive from this discussion desirable properties for integral transforms to be useful in this context. In Section 3 we shall give the general prescription for the evaluation of the kernel equation (1.2) by the use of integral transforms. In Section 4 explicit expressions are given using the H-transform and assuming all clusters to be made up of ${}^1S$ oscillator functions of arbitrary width. In Section 5 finally we discuss the possibility of a group theoretical interpretation of the method presented and the usefulness of such interpretations.

Part of the results discussed here are contained in the Ph.D. Thesis of one of us (W.Z.) [10].

2. The H-transform

Consider the function [15]

$$f_\vartheta(x, k) = \pi^{-1/2} \exp\left\{-\tfrac{1}{2}\vartheta x^2 + 2ikx + \frac{1}{\vartheta} k^2\right\} \tag{2.1}$$

of the variables x and k both ranging over $\mathbb{R}$. If we consider $f_\vartheta(x, k)$ as a generating function for harmonic oscillator functions

$$\varphi_n(\sqrt{\vartheta}\, x) = \left(\frac{\vartheta^{1/2}}{\pi^{1/2} 2^n n!}\right)^{1/2} H_n(\sqrt{\vartheta}\, x)\, e^{-1/2\vartheta x^2} \tag{2.2}$$

where H_n are Hermite polynomials, we have [16]

$$f_\vartheta(x, k) = \pi^{-1/4} \sum_n k^n (-2)^{n/2} (\vartheta^{n-1} n!)^{-1/2} \varphi_n(\sqrt{\vartheta}\, x). \tag{2.3}$$

We shall now reinterpret $f_\vartheta(x, k)$ as an integral transform such that

$$\psi(x) = \int f_\vartheta(x, k) g(k)\, dk. \tag{2.4}$$

The measure in k-space is chosen arbitrarily to be dk. This is very convenient for computations but needs justification. We use a criterion for the applicability of integral transforms in many-body problems derived elsewhere [17]. Apart from some questions of integrability that are always fulfilled for the Gaussians we use, this criterion requires that an integral transform must map a dense subspace of $\mathscr{L}^2(\mathbb{R})$ into a dense subspace of some other Hilbertspace, that in our case we wish to be $\mathscr{L}^2(\mathbb{R})$ again. This is indeed the case as we have

$$\int f_\vartheta(x, k) \gamma^{1/2} e^{-\gamma k^2}\, dk = \left(\frac{\rho - \vartheta}{2\vartheta}\right)^{1/2} e^{-1/2\rho x^2}$$

$$\rho = \vartheta \frac{\gamma + 1/\vartheta}{\gamma - 1/\vartheta}; \qquad 1/\vartheta < \gamma < \infty. \tag{2.5}$$

The restriction $1/\vartheta < \gamma < \infty$ ensures convergence of the integral and entails $\vartheta < \rho < \infty$. For $\gamma < 1/\vartheta$ the integral diverges and thus the integral transform is singular, i.e., the corresponding operator is unbounded. According to Reference [17] this is of no consequence as the Gaussians with width parameters between a fixed point and infinity span dense subsets of $\mathscr{L}^2(\mathbb{R})$.

The integral in (2.5) would also converge with any finite polynomial in k preceding the Gaussian and yield some other polynomial in x. We may therefore identify the dense subspaces of $\mathscr{L}^2(\mathbb{R})$ involved as spaces of functions of exponential growth smalller than $[2, -1/\vartheta]$ or $[2, -\frac{1}{2}\vartheta]$, i.e., of functions decreasing more rapidly than $\exp[-1/\vartheta\, k^2]$ and $\exp[-\frac{1}{2}\vartheta x^2]$. On the image space we may now also define an inverse transform

$$\int f_\vartheta^{-1}(x, k)\, \psi(x) = g(k) \tag{2.6}$$

with

$$f_\vartheta^{-1}(x, k) = \pi^{-1/2} \exp\left\{\frac{1}{2}\vartheta x^2 - 2ikx - \frac{1}{\vartheta}k^2\right\}. \tag{2.7}$$

It can readily be checked explicitly that this transform converges if applied to functions of exponential growth less than $[2, -1/2\vartheta]$. Thus this integral transform is acceptable and its 'inverse' exists in the sense discussed above. Simultaneously we can use its generating function property to evaluate matrix elements of some operator Op between oscillator functions of arbitrary width as

$$\begin{aligned}\int \varphi_{\bar{n}}^*(\sqrt{\bar{\vartheta}}\, x)\, \mathrm{Op}\, \varphi_n(\sqrt{\vartheta}\, x)\, dx \\ &= \left[\left(\frac{\partial}{\partial \bar{k}}\right)^{\bar{n}}\left(\frac{\partial}{\partial k}\right)^{n}\left\{\int f_{\bar{\vartheta}}^*(\bar{k}, x)\, \mathrm{Op}\, f_\vartheta(k, x)dx\right\}\right]_{\bar{k}=0,\, k=0} \\ &= \left[\left(\frac{\partial}{\partial \bar{k}}\right)^{\bar{n}}\left(\frac{\partial}{\partial k}\right)^{n}\{H(\bar{k}, k)\}\right]_{\bar{k}=0, k=0}\end{aligned} \tag{2.8}$$

Here $H(\bar{k}, k)$ is the kernel of an integral transform representing the action of Op between spaces over the variables $\bar{k}$ and k. Knowing this kernel we are thus in a position to evaluate oscillator matrix elements in a very simple way.

Note that this kernel does not correspond to the transform of an operator in the usual sense: This not only because we may have $\bar{\vartheta} \neq \vartheta$ but mainly because we have

$$f_\vartheta^*(k, x) \neq f_\vartheta^{-1}(k, x). \tag{2.9}$$

While the relations

$$\int f_\vartheta^{-1}(\bar{k}, x) f_\vartheta(k, x)\, dx = \delta(\bar{k} - k) \tag{2.10a}$$

$$\int f_\vartheta^{-1}(k, \bar{x}) f_\vartheta(k, x)\, dk = \delta(\bar{x} - x) \tag{2.10b}$$

must hold, the kernel associated with the identity is given by

$$\begin{aligned}\int f_{\bar{\vartheta}}^*(\bar{k}, x) f_\vartheta(k, x)\, dx = \pi^{1/2}\left(\frac{\bar{\vartheta} + \vartheta}{2}\right)^{-1/2} \\ \exp\left\{\left(\frac{1}{\bar{\vartheta}} - \frac{2}{\bar{\vartheta} + \vartheta}\right)\bar{k}^2 + \left(\frac{4}{\bar{\vartheta} + \vartheta}\right)\bar{k}k + \left(\frac{1}{\vartheta} - \frac{2}{\bar{\vartheta} + \vartheta}\right)k^2\right\}.\end{aligned} \tag{2.11}$$

This integral exists for any choice of $\bar{\vartheta}$ and ϑ and therefore the kernel corresponding to the unit operator never contains a Dirac δ. It is readily checked that no Dirac δ's

appear for any of the other operators of interest. The integral transform thus shows the desired features and we merely have to extend it to m dimensions. We do this simply by taking a product kernel as

$$F(\mathbf{k}, \mathbf{x}) = \prod_{i=1}^{m} f_{\vartheta_i}(k_i, x_i) = \pi^{-m/2} \exp\left\{-\frac{1}{2}\mathbf{x}^t D\mathbf{x} + 2i\mathbf{x}^t\mathbf{k} + \mathbf{k}^t D^{-1}\mathbf{k}\right\}. \quad (2.12)$$

Here $\mathbf{x}$, $\mathbf{k}$ are m-dimensional column vectors and D is a diagonal matrix with elements ϑ_i. The matrix notation in the last line is introduced for later convenience with t denoting transposition throughout this paper.

We shall call the integral transform with the kernel given in (2.12) H-transform. In this form it was first used in Reference [10] and it constitutes a generalization of the one used in Reference [15] where the case of all ϑ_i being equal was considered. From (2.8) it is obvious that the transform (2.12) can be used to generate matrix elements between functions of two different m-dimensional anisotropic oscillators.

We may now ask what features of the H-transform are particularly important and we shall see that they are the following three:

(1) The H-transform possesses an 'inverse', and the representation of the problem in the new space is thus unique.
(2) The H-transform has generating function properties and thus allows simple evaluation of matrix elements.
(3) The H-transform is Gaussian and of simple product form. This allows analytic evaluation of integrals and a relatively simple treatment of orthogonal transformations (including permutations).

3. The construction of the kernel

To construct the kernel we shall proceed in three steps. As it will prove convenient to use three systems of coordinates we shall start by presenting them and fixing the notation to avoid confusion.

The three systems are illustrated in Figure 1 using the example of five nucleons partitioned into two clusters. We shall refer to them as single particle (a), single cluster (b) and generalized Jacobi coordinates (c). Further we shall use the terms cluster c.m. and mode coordinates if in the situation illustrated by (b) and (c) we wish to disregard the internal variables of the clusters. Note that the figures serve as illustration only as we shall use orthogonal transformations to connect the systems. In the first line of Table I we list the symbols associated with the different coordinates. As mentioned above the lower index refers to the three space components whereas the upper index (ranging from 1 to n or 1 to κ) indicates the variable. Bold face is to indicate collections of the variables to an n or κ dimensional column vector while an arrow indicates a three dimensional vector in space. The transformations between the three coordinate systems may be performed for each space component separately and read as

$$\mathbf{s}_i = O_{\mathrm{I}}^t \mathbf{x}_i, \qquad \mathbf{r}_i = O_{\mathrm{II}}^t \mathbf{s}_i; \quad i = 1, 2, 3. \quad (3.1)$$

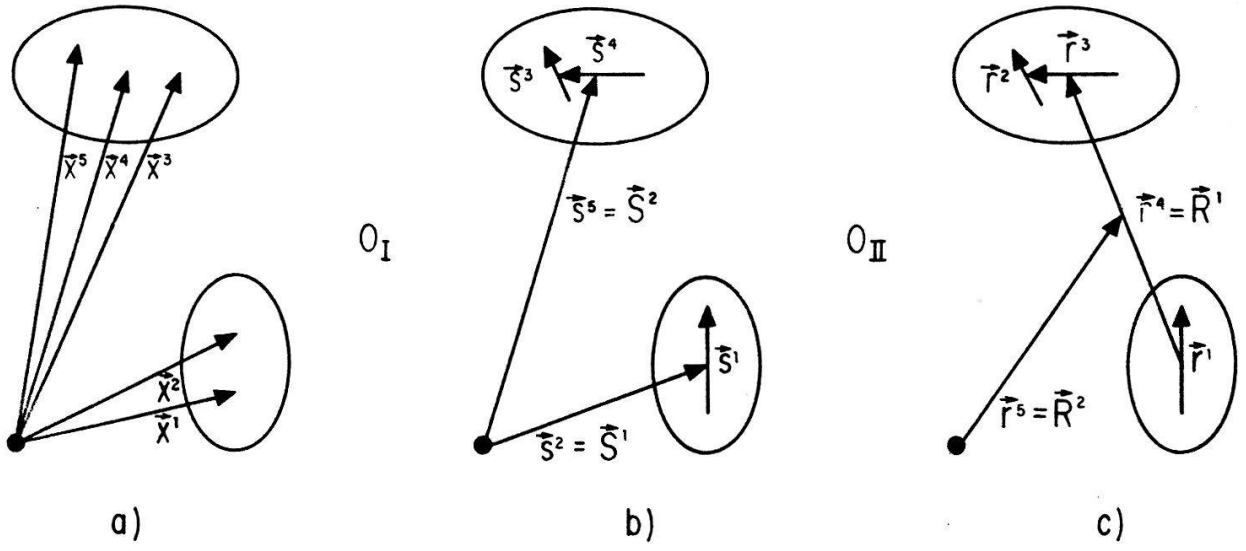

Figure 1
The three coordinate systems illustrated for a five-particle system.

Table I
Variables in configuration space and in the transformed space

	Coordinates				
Space	Single particle	Single cluster	Cluster c.m.	Generalized Jacobi	Cluster mode
Configuration	$\vec{\mathbf{x}}$	$\vec{\mathbf{s}}$	$\vec{\mathbf{S}}$	$\vec{\mathbf{r}}$	$\vec{\mathbf{R}}$
Transformed	$\vec{\mathbf{k}}$	$\vec{\mathbf{t}}$	$\vec{\mathbf{T}}, \vec{\mathbf{V}}$		$\vec{\mathbf{Q}}$

O_{II} does not affect the internal variables of the clusters and therefore no confusion should arise as we write loosely

$$\mathbf{R}_i = O_{II}^t \mathbf{S}_i. \tag{3.2}$$

We shall write the integral transform in single particle coordinates. For this purpose we give the diagonal matrix

$$A = \begin{bmatrix} \overbrace{\alpha_1 \cdots \alpha_1}^{n_1} & & \overbrace{\alpha_K \cdots \alpha_K}^{n_K} \end{bmatrix}, \tag{3.3}$$

where α_i is the width parameter associated with the internal function of the ith cluster φ_i. Using (2.12) we then write the kernel as

$$F(\vec{\mathbf{k}}, \vec{\mathbf{x}}) = \pi^{-3n/2} \prod_{i=1}^{3} \exp\{-\tfrac{1}{2}\mathbf{x}_i^t A \mathbf{x}_i + 2i\mathbf{x}_i^t \mathbf{k}_i + \mathbf{k}_i^t A^{-1} \mathbf{k}_i\} \tag{3.4}$$

where $\vec{\mathbf{k}}$ indicates the transformed single particle variables, listed in the second line of Table I. Using this notation we can transform our initial operator $\bar{P}$ Op P to an integral transform between the $\bar{\vec{\mathbf{k}}}$ and the $\vec{\mathbf{k}}$ space with the kernel

$$H(\bar{\vec{\mathbf{k}}}, \vec{\mathbf{k}}) = \int\int \bar{F}^*(\bar{\vec{\mathbf{k}}}, \vec{\mathbf{x}})\bar{P} \text{ Op } PF(\vec{\mathbf{k}}, \vec{\mathbf{x}})\, d\vec{\mathbf{x}}. \tag{3.5}$$

The integral can be performed readily in closed form for operators made up of Gaussians, powers and spherical harmonics. In the next section we shall give explicit expressions for the norm and two-body operators. This completes the first step eliminating all Dirac δ's from the procedure.

Next, using

$$[O_{\mathrm{I}}, A] = 0, \qquad [O_{\mathrm{II}}, A] \neq 0 \tag{3.6}$$

it is easy to see from equation (3.1) that we could have written equation (3.4) equally in single cluster coordinates with transformed variables

$$\mathbf{t}_i = O_{\mathrm{I}}^t \mathbf{k}_i; \quad i = 1, 2, 3 \tag{3.7}$$

whereas the same would not have been possible for generalized Jacobi coordinates. For this reason we choose to perform the integration over internal variables in single cluster coordinates in which the kernel reads as

$$\begin{aligned} L(\bar{\vec{\mathbf{t}}}, \vec{\mathbf{t}}) &= L(\bar{\mathbf{t}}_1, \bar{\mathbf{t}}_2, \bar{\mathbf{t}}_3; \mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3) \\ &= H(\bar{O}_{\mathrm{I}}\bar{\mathbf{t}}_1, \bar{O}_{\mathrm{I}}\bar{\mathbf{t}}_2, \bar{O}_{\mathrm{I}}\bar{\mathbf{t}}_3; O_{\mathrm{I}}\mathbf{t}_1, O_{\mathrm{I}}\mathbf{t}_2, O_{\mathrm{I}}\mathbf{t}_3). \end{aligned} \tag{3.8}$$

Now we may apply the generating function properties of $\bar{F}$ and F to perform in a trivial way the integration over internal variables resulting in a kernel

$$\mathscr{H}(\bar{\vec{\mathbf{T}}}, \vec{\mathbf{T}}) = l(\bar{\vec{\mathbf{T}}}, \vec{\mathbf{T}})L(\bar{\vec{\mathbf{T}}}, \vec{\mathbf{T}}). \tag{3.9}$$

Here $\vec{\mathbf{T}}$ represents the transformed cluster c.m. variables that are merely a subset of the $\vec{\mathbf{t}}$ (Table I). L is the same kernel as in (3.8) except that the internal variables have been set equal to zero, and l is the polynominal that resulted from differentiating the variables of the generating function to obtain the integration over the cluster functions φ_i. We refer to this process as freezing of the internal coordinates in a given state.

In some cases, particularly for closed shells it may be convenient to perform the differentiation in single particle coordinates and perform the orthogonal transformation thereafter. This procedure indicates the relation to the Hill–Wheeler method [9], where the kernel equation (3.5) is evaluated by techniques related to the Slater determinant method for single particle functions [6].

In the next section the kernel (3.9) is given explicitly for the case of an arbitrary number of ^1S shell clusters. In this case the term l will not appear. Thus step 2, the integration over the internal variables, is completed and we have obtained the kernel in cluster c.m. variables.

The last step is now to obtain the kernel in cluster mode variables. We may choose whether we wish the kernel in the original variables $\vec{\mathbf{R}}$ or in a set of transformed variables. In the first case obviously the Dirac δ's will appear again, but also the second possibility is nontrivial because the corresponding variables are not related to $\vec{\mathbf{T}}$ by an orthogonal transformation due to the different parameters α_i involved for each $\vec{T}^i$. We must therefore consider the inverse transform acting on the variables $\bar{\vec{\mathbf{T}}}$

defined by the kernel

$$G^{-1}(\vec{\mathbf{T}}, \vec{\mathbf{S}}) = \pi^{-3\kappa/2} \prod_{i=1}^{3} \exp\{\tfrac{1}{2}\mathbf{S}_i^t B \mathbf{S}_i - 2i\mathbf{S}_i^t \mathbf{T}_i - \mathbf{T}_i^t B^{-1} \mathbf{T}_i\} \tag{3.10}$$

with the diagonal matrix

$$B = \begin{bmatrix} \alpha_1 & & & \\ & \alpha_2 & & \\ & & \ddots & \\ & & & \alpha_\kappa \end{bmatrix}. \tag{3.11}$$

We could then write the kernel

$$\mathscr{K}'(\bar{\vec{\mathbf{S}}}, \vec{\mathbf{S}}) = \int\int \bar{G}^{-1*}(\bar{\vec{\mathbf{T}}}, \bar{\vec{\mathbf{S}}}) \mathscr{H}(\bar{\vec{\mathbf{T}}}, \vec{\mathbf{T}}) G^{-1}(\vec{\mathbf{T}}, \vec{\mathbf{S}}) \tag{3.12}$$

and finally obtain the kernel (1.2) in the original space as

$$\begin{aligned} \mathscr{K}(\bar{\vec{\mathbf{R}}}, \vec{\mathbf{R}}) &= \mathscr{K}(\bar{\mathbf{R}}_1, \bar{\mathbf{R}}_2, \bar{\mathbf{R}}_3; \mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3) \\ &= \mathscr{K}'(\bar{O}_{\text{II}}\bar{\mathbf{R}}_1, \bar{O}_{\text{II}}\bar{\mathbf{R}}_2, \bar{O}_{\text{II}}\bar{\mathbf{R}}_3; O_{\text{II}}\mathbf{R}_1, O_{\text{II}}\mathbf{R}_2, O_{\text{II}}\mathbf{R}_3). \end{aligned} \tag{3.13}$$

As mentioned above this kernel will sometimes contain Dirac δ's and if we wish to avoid this we may define another transform

$$G_0(\vec{\mathbf{S}}, \vec{\mathbf{V}}) = \pi^{-3\kappa/2} \prod_{i=1}^{3} \exp\{-\tfrac{1}{2}\beta \mathbf{S}_i^t I \mathbf{S}_i + 2i\mathbf{S}_i^t \mathbf{V}_i + \beta^{-1} \mathbf{V}_i^t I \mathbf{V}_i\} \tag{3.14}$$

where $\beta < \max(\alpha_i)$ is some constant, I the unit $\kappa \cdot \kappa$ matrix and $\vec{\mathbf{V}}$ is a second set of transformed variables related to $\vec{\mathbf{S}}$ by G_0 rather than G. G_0 could have been equally written in terms of the cluster mode variables $\vec{\mathbf{R}}$ and $\vec{\mathbf{Q}}$ if we define

$$\mathbf{Q}_i = O_{\text{II}}^t \mathbf{V}_i; \quad i = 1, 2, 3. \tag{3.15}$$

We may now combine the transforms equations (3.14) and (3.10) to yield the kernel

$$\begin{aligned} \Gamma(\vec{\mathbf{T}}, \vec{\mathbf{V}}) &= \int G^{-1}(\vec{\mathbf{T}}, \vec{\mathbf{S}}) G_0(\vec{\mathbf{V}}, \vec{\mathbf{S}})\, d\vec{\mathbf{S}} \\ &= \pi^{-3\kappa/2} \left| \det\left(\frac{\beta I - B}{2}\right) \right|^{-3/2} \prod_{i=1}^{3} \exp\{-\mathbf{T}_i^t B^{-1} \mathbf{T}_i + \beta^{-1} \mathbf{V}_i^t I \mathbf{V}_i\} \\ &\qquad \exp\{-2(\mathbf{V}_i - \mathbf{T}_i)^t (\beta I - B)^{-1} (\mathbf{V}_i - \mathbf{T}_i)\} \end{aligned} \tag{3.16}$$

Due to the restrictions on β this integral always converges and we write

$$\mathscr{M}(\bar{\vec{\mathbf{V}}}, \vec{\mathbf{V}}) = \int\int \bar{\Gamma}^{*}(\bar{\vec{\mathbf{V}}}, \bar{\vec{\mathbf{T}}}) \mathscr{H}(\bar{\vec{\mathbf{T}}}, \vec{\mathbf{T}}) \Gamma(\vec{\mathbf{V}}, \vec{\mathbf{T}})\, d\bar{\vec{\mathbf{T}}}\, d\vec{\mathbf{T}} \tag{3.17}$$

and finally obtain the kernel in transformed cluster c.m. coordinates as

$$\begin{aligned} \mathscr{N}(\bar{\vec{\mathbf{Q}}}, \vec{\mathbf{Q}}) &= \mathscr{N}(\bar{\mathbf{Q}}_1, \bar{\mathbf{Q}}_2, \bar{\mathbf{Q}}_3; \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3) \\ &= \mathscr{M}(\bar{O}_{\text{II}}\bar{\mathbf{Q}}_1, \bar{O}_{\text{II}}\bar{\mathbf{Q}}_2, \bar{O}_{\text{II}}\bar{\mathbf{Q}}_3; O_{\text{II}}\mathbf{Q}_1, O_{\text{II}}\mathbf{Q}_2, O_{\text{II}}\mathbf{Q}_3). \end{aligned} \tag{3.18}$$

The integral in (3.17) can be done analytically by completing squares under the same conditions under which $\mathscr{H}$ was obtained. Yet explicit expressions are not available

in a general form because the matrix inversion involved is nontrivial; on the other hand the problem at this stage involves only matrices of dimension $\bar{\kappa}$ or κ rather than n and is thus more amenable to any kind of treatment and of the same order of difficulty as the integrations which remain anyway.

We may add that in the oscillator limit $\alpha_i = \alpha$ the last step becomes trivial and we obtain

$$\begin{aligned}\mathcal{N}_{\text{osc.}}(\bar{\vec{\mathbf{Q}}}, \vec{\mathbf{Q}}) &= \mathcal{N}_{\text{osc.}}(\bar{\mathbf{Q}}_1, \bar{\mathbf{Q}}_2, \bar{\mathbf{Q}}_3; \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3) \\ &= \mathcal{H}(\bar{O}_{\text{II}}\bar{\mathbf{Q}}_1, \bar{O}_{\text{II}}\bar{\mathbf{Q}}_2, \bar{O}_{\text{II}}\bar{\mathbf{Q}}_3; O_{\text{II}}\mathbf{Q}_1, O_{\text{II}}\mathbf{Q}_2, O_{\text{II}}\mathbf{Q}_3). \qquad (3.19)\end{aligned}$$

Note that only the general properties of the H-transform mentioned at the end of Section 2 are actually needed to perform the steps indicated in this section.

While the generating function technique is very effective to perform the integrations over internal variables, other methods are conceivable. As mentioned above the Hill–Wheeler method obtains the result (3.9) in a different way but the procedure to overcome the oscillator limit from there on would be the same.

4. Closed expressions for the kernels in cluster C.M. coordinates

In this section we shall show how to implement by explicit expressions steps 1 and 2 which we mentioned in the last chapter.

We shall consider two-body operators such as central, spin-orbit and tensor interactions with Gaussian wells as well as the kinetic energy in relative coordinates. The unit operator relevant for the norm will also be considered. The treatment of these operators suffices to perform a resonating group calculation as the Coulomb interaction may effectively be expanded into a superposition of Gaussians [18] and an adequate phenomenological nucleon–nucleon potential is given in the corresponding form [19]. Approximations simulating short-range correlations are also possible in this framework [20]. The details involving the terms of the interactions do not enter the general argument and appear only in Appendix 1.

For two-body operators the expression $\bar{P}$ Op P (2.2) can be written in the form [8]

$$\bar{Z}T_{(n-1,\,n)}Z'Z''Z. \qquad (4.1)$$

Herein $T_{(n-1,\,n)}$ is the term of the two-body operator which acts on the relative motion vector of particles $(n-1)$ and n. $\bar{Z}$, Z are permutations which determine the interacting particles in bra and ket respectively, Z' gives the permutation of the $(n-2)$ non-interacting and Z'' the permutation of the interacting particles. Note that

$$[Z', T_{(n-1,\,n)}] = [Z'', T_{(n-1,\,n)}] = 0.$$

For step 1 we are then interested in the determination of

$$\int \bar{F}^*(\bar{\vec{\mathbf{k}}}, \vec{\mathbf{x}})\bar{Z}T_{(n-1,\,n)}Z'Z''ZF(\vec{\mathbf{k}}, \vec{\mathbf{x}})\, d\vec{\mathbf{x}}. \qquad (4.2)$$

First we shall consider the simple problem of a norm term where $T_{(n-1,\,n)} = I$ (identity) and we write the product of permutations as one permutation P. We then see immediately by completing squares and identifying permutations with permutation matrices that

$$
\begin{aligned}
H(\bar{\vec{\mathbf{k}}}, \vec{\mathbf{k}}) &= \prod_{i=1}^{3} \int \bar{F}^*(\mathbf{x}_i, \bar{\mathbf{k}}_i) P F(\mathbf{x}_i, \mathbf{k}_i)\, d\mathbf{x}_i \\
&= \prod_{i=1}^{3} \int \bar{F}^*(\mathbf{x}_i, \bar{\mathbf{k}}_i) F(P^t\mathbf{x}_i, \mathbf{k}_i)\, d\mathbf{x}_i \\
&= \pi^{-3n} \prod_{i=1}^{3} \exp\{\bar{\mathbf{k}}_i^t \bar{A}^{-1} \bar{\mathbf{k}}_i + \mathbf{k}_i^t A^{-1} \mathbf{k}_i\} \\
&\qquad \int d\mathbf{x}_i \exp\{-\tfrac{1}{2}\mathbf{x}_i^t(\bar{A} + {}^P A)\mathbf{x}_i + 2i\mathbf{x}_i^t(P\mathbf{k}_i - \bar{\mathbf{k}}_i)\} \\
&= \left\{\pi^{-n} \det\left(\frac{\bar{A} + {}^P A}{2}\right)\right\}^{-3/2} \prod_{i=1}^{3} \exp\left\{\bar{\mathbf{k}}_i^t \left(\bar{A}^{-1} - \left(\frac{\bar{A} + {}^P A}{2}\right)^{-1}\right)\bar{\mathbf{k}}_i \right. \\
&\quad \left. + 2\bar{\mathbf{k}}_i^t \left(\frac{\bar{A} + {}^P A}{2}\right)^{-1} P\mathbf{k}_i + \mathbf{k}_i^t \left(A^{-1} - \left(\frac{{}^{P^t}\bar{A} + A}{2}\right)^{-1}\right)\mathbf{k}_i\right\} \\
&= \left\{\pi^{-n} \det\left(\frac{\bar{A} + {}^P A}{2}\right)\right\}^{-3/2} \prod_{i=1}^{3} \exp\{\bar{\mathbf{k}}_i^t R \bar{\mathbf{k}}_i + 2\bar{\mathbf{k}}_i^t S \mathbf{k}_i + \mathbf{k}_i^t T \mathbf{k}_i\} \qquad (4.3)
\end{aligned}
$$

where for any matrix Λ we write $P\Lambda P^t = {}^P\Lambda$. Note that ${}^P\Lambda$ is diagonal if Λ is diagonal. All matrix inversions in (4.3) are trivial and R, S and T in the last line are given by trivial matrix operations. Thus step 1 is completed for the norm. Note further that the kernel separates completely as the matrices R and T are diagonal and S is a diagonal matrix multiplied by a permutation matrix, i.e., the kernel could be written as a product of single particle kernels.

In general this is no longer true as $T_{(n-1,\,n)}$ will contain mixed terms in the coordinates of particles $(n-1)$ and n. However, we still expect the kernel to factorize up to two coordinates. Actually we are able to factorize the kernel into an $(n-2)$-particle norm factor and a two-body interaction factor. To do this in the matrix notation adopted here we introduce the matrices

$$
M' = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ 0 & & & 0 & \\ & & & & 0 \end{pmatrix}, \qquad M'' = \begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ 0 & & & 1 & \\ & & & & 1 \end{pmatrix}. \qquad (4.4)
$$

In order to evaluate (4.2) we factorize

$$
ZF(\bar{\vec{\mathbf{x}}}, \vec{\mathbf{k}}) = \pi^{-3n/2} \prod_{i=1}^{3} \exp\{-\tfrac{1}{2}\mathbf{x}_i^t {}^Z A \mathbf{x}_i + 2i\mathbf{x}_i^t Z \mathbf{k}_i + \mathbf{k}_i^t A^{-1} \mathbf{k}_i\} = F'F'' \qquad (4.5)
$$

with

$$
\begin{aligned}
F' &= \pi^{-3(n-2)/2} \prod_{i=1}^{3} \exp\{-\tfrac{1}{2}\mathbf{x}_i^t M'^Z A M' \mathbf{x}_i + 2i\mathbf{x}_i^t M' Z \mathbf{k}_i \\
&\quad + \mathbf{k}_i^t {}^{Z^t}M' A^{-1\,Z^t} M' \mathbf{k}_i\} \\
F'' &= \pi^{-3} \prod_{i=1}^{3} \exp\{-\tfrac{1}{2}\mathbf{x}_i^t M''^Z A M'' \mathbf{x}_i + 2i\mathbf{x}_i^t M'' Z \mathbf{k}_i \\
&\quad + \mathbf{k}_i^t {}^{Z^t}M'' A^{-1\,Z^t} M'' \mathbf{k}_i\}. \qquad (4.6)
\end{aligned}
$$

We want to underline at this point once more the significance of this factorization: F' contains only variables x_i^s and $k_i^{Z(s)}$, $s = 1, \ldots, n-2$; $i = 1, 2, 3$ and F'' contains only x_i^{n-1}, $k_i^{Z(n-1)}$, x_i^n and $k_i^{Z(n)}$; $i = 1, 2, 3$.

Here $Z(s)$ is the index into which s is transformed by the permutation Z. Defining $\bar{F}'$ and $\bar{F}''$ similarly we have

$$\int \bar{F}^*(\vec{\bar{\mathbf{k}}}, \vec{\bar{\mathbf{x}}}) \bar{Z} T_{(n-1,n)} Z' Z'' Z F(\vec{\mathbf{k}}, \vec{\mathbf{x}}) = \left\{ \int \bar{F}' Z' F' \prod_{i=1}^{3} \prod_{s=1}^{n-2} dx_i^s \right\} \left\{ \int \bar{F}'' T_{(n-1,n)} Z'' F'' \prod_{i=1}^{3} dx_i^{n-1} \, dx_i^n \right\}. \quad (4.7)$$

The factors in the two brackets commute and hence can be evaluated separately. The first term represents exactly a $(n-2)$-particle norm problem similar to the one whose solution is given in (4.3) but with the two interacting particles removed from the corresponding clusters. On the other hand

$$\int \bar{F}'' T_{(n-1,n)} Z'' F'' \prod_{i=1}^{3} dx_i^{n-1} \, dx_i^n = H''(\vec{\bar{k}}^{\bar{Z}(n-1)}, \vec{\bar{k}}^{\bar{Z}(n)}; \vec{k}^{Z''Z(n-1)}, \vec{k}^{Z''Z(n)}) \quad (4.8)$$

is a kernel involving only two particles that can be evaluated analytically. The kernels H'' for the relevant operators are given in Appendix 1. We have thus completed the first step described in the previous section; the integral kernels in $\vec{\bar{\mathbf{k}}}$ and $\vec{\mathbf{k}}$ corresponding to the relevant operators are available explicitly. We shall now perform the second step associated with equations (3.8), (3.9) for the special case that all clusters are described by ^1S oscillator functions. As mentioned this implies that the term $l(\vec{\bar{\mathbf{T}}}, \vec{\mathbf{T}})$ of (3.9) does not appear. We therefore have to pass to single cluster coordinates and retain only the terms in cluster c.m. coordinates.

It is advantageous not to calculate the terms in (3.8) that will be dropped by setting the internal cluster coordinates equal to zero. This is possible if we keep in mind that $T_i^\mu = 1/\sqrt{n_\mu}\, {}^\mu\!\sum_s k_i^s$ where the sum ${}^\mu\!\sum_s$ runs over all particle indices in cluster μ. This implies that we find the coefficient for $\bar{T}_i^{\bar{\mu}} \, T_i^\mu$ if we collect all coefficients of terms $\bar{k}_i^s k_i^r$ with particle s belonging to cluster $\bar{\mu}$ on the left and particle r to cluster μ on the right side. These coefficients must be summed and divided by $\sqrt{\bar{n}_{\bar{\mu}} n_\mu}$; obviously this has to be done separately for exponents and polynominals. We may proceed similarly for terms in $T_i^\mu \, T_i^\nu$ and $\bar{T}_i^{\bar{\mu}} \, \bar{T}_i^{\bar{\nu}}$.

We shall again first consider the norm, but now use the concept of double coset (DC) symbols [8] which are also known as coarse permutation matrices [4]. A DC-symbol is a $\bar{\kappa} \cdot \kappa$ matrix with elements $d_{\bar{\mu},\mu}$ defined as

$$d_{\bar{\mu},\mu} = {}^{\bar{\mu}}\!\sum_s \, {}^{\mu}\!\sum_r P_{s,r} \quad (4.9)$$

where $P_{s,t}$ are the elements of the permutation matrix P.

As it was shown in Reference [8] all permutations having the same DC-symbol will yield the same matrix elements and indeed $d_{\bar{\mu},\mu}$ gives the number of particles permuted from cluster μ to cluster $\bar{\mu}$ by P. If we now wish to find the coefficient of $\bar{T}_i^{\bar{\mu}} \, T_i^\mu$ according to the prescription given above, we have to concentrate on the matrix S in (4.3). It is apparent that each contributing term has a coefficient that is

either zero or $4/(\bar{\alpha}_{\bar{\mu}} + \alpha_\mu)$. The number of such terms is the number of particles taken from cluster μ to cluster $\bar{\mu}$, i.e., $d_{\bar{\mu},\mu}$ and thus the coefficient of $\bar{T}_i^{\bar{\mu}}\, T_i^{\mu}$ in the exponent is $4\, d_{\bar{\mu},\mu}[(\bar{\alpha}_{\bar{\mu}} + \alpha_\mu)\sqrt{\bar{n}_{\bar{\mu}}}\sqrt{n_\mu}]^{-1}$. The other coefficients may be found by similar considerations and we obtain the final result in matrix notation as

$$\mathscr{H}(\bar{\bar{\mathbf{T}}}, \vec{\mathbf{T}}) = \pi^{3n/2} \left| \prod_{\bar{\mu},\mu=1}^{\bar{\kappa},\kappa} \left(\frac{\bar{\alpha}_{\bar{\mu}} + \alpha_\mu}{2} \right)^{d_{\bar{\mu},\mu}} \right|^{-3/2} \prod_{i=1}^{3} \exp\{\bar{\mathbf{T}}_i^t \rho \bar{\mathbf{T}}_i + \bar{\mathbf{T}}_i^t \sigma \mathbf{T}_i + \mathbf{T}_i^t \tau \mathbf{T}_i\} \tag{4.10}$$

where ρ, σ and τ are matrices with elements

$$\rho_{\bar{\mu},\bar{\nu}} = \left(-\sum_{\mu=1}^{\kappa} 2\, d_{\bar{\mu},\mu} (\bar{\alpha}_{\bar{\mu}} + \alpha_\mu)^{-1} + \bar{n}_{\bar{\mu}} \bar{\alpha}_{\bar{\mu}}^{-1} \right) \frac{\delta_{\bar{\mu},\bar{\nu}}}{\bar{n}_{\bar{\mu}}} \tag{4.11a}$$

$$\sigma_{\bar{\mu},\mu} = 4\, d_{\bar{\mu},\mu} (\bar{\alpha}_{\bar{\mu}} + \alpha_\mu)^{-1} \frac{1}{\sqrt{\bar{n}_{\bar{\mu}}}\sqrt{n_\mu}} \tag{4.11b}$$

$$\tau_{\mu,\nu} = \left(-\sum_{\bar{\mu}=1}^{\bar{\kappa}} 2\, d_{\bar{\mu},\mu} (\bar{\alpha}_{\bar{\mu}} + \alpha_\mu)^{-1} + n_\mu \alpha_\mu^{-1} \right) \frac{\delta_{\mu,\nu}}{n_\mu} \tag{4.11c}$$

for the norm. In the oscillator limit where the width parameters $\bar{\alpha}_{\bar{\mu}} = \alpha_\mu = \alpha$ are all equal, equations (4.10, 11) reduce to

$$\mathscr{H}_{\text{osc.}}(\bar{\bar{\mathbf{T}}}, \vec{\mathbf{T}}) = \left(\frac{\pi}{\alpha}\right)^{3n/2} \prod_{i=1}^{3} \exp\left\{\frac{2}{\alpha} \bar{\mathbf{T}}_i^t \sigma \mathbf{T}_i\right\},\ \sigma_{\bar{\mu},\mu} = \frac{d_{\bar{\mu},\mu}}{\sqrt{\bar{n}_{\bar{\mu}} n_\mu}}. \tag{4.12}$$

For two-particle operators we shall start from the factorization (4.7) and introduce explicitly the transformation (3.8) for the two-particle kernel

$$\mathscr{H}''(\bar{\bar{T}}^{\bar{\mu}(\bar{Z}(n-1))}, \bar{\bar{T}}^{\bar{\mu}(\bar{Z}(n))}; \vec{T}^{\mu(Z''Z(n-1))}, \vec{T}^{\mu(Z''Z(n))})$$
$$= H''\left(\frac{\bar{\bar{k}}^{\bar{Z}(n-1)}}{\sqrt{\bar{n}_{\bar{\mu}(\bar{Z}(n-1))}}}, \frac{\bar{\bar{k}}^{\bar{Z}(n)}}{\sqrt{\bar{n}_{\bar{\mu}(\bar{Z}(n))}}}; \frac{\vec{k}^{Z(n-1)}}{\sqrt{n_{\mu(Z''Z(n-1))}}}, \frac{\vec{k}^{Z(n)}}{\sqrt{n_{\mu(Z''Z(n))}}} \right). \tag{4.13}$$

Here $\mu(s)$ is the cluster in which particle s is located. The first factor in (2.7) is a $(n-2)$-particle norm term given by (4.10) if we replace P by Z'. We can then write down the closed expression

$$\mathscr{H}(\bar{\bar{\mathbf{T}}}, \vec{\mathbf{T}}) = \pi^{3n/2} \left| \prod_{\bar{\mu},\mu=1}^{\bar{\kappa},\kappa} \left(\frac{\bar{\alpha}_{\bar{\mu}} + \alpha_\mu}{2} \right)^{d_{\bar{\mu},\mu}} \right|^{-3/2} \prod_{i=1}^{3} \exp\{\bar{\mathbf{T}}_i^t \rho' \bar{\mathbf{T}}_i + \bar{\mathbf{T}}_i^t \sigma' \mathbf{T}_i + \mathbf{T}_i^t \tau' T_i\}$$
$$\mathscr{H}''(\bar{\bar{T}}^{\bar{\mu}(\bar{Z}(n-1))}, \bar{\bar{T}}^{\bar{\mu}(\bar{Z}(n))}; \vec{T}^{\mu(Z(n-1))}, \vec{T}^{\mu(Z(n))}) \tag{4.14}$$

thus completing step 2. The matrices ρ', σ', τ' are obtained from the equations (4.11a, b, c) for ρ, σ, τ by replacing in those expressions $d_{\bar{\mu},\mu}$ by $d'_{\bar{\mu},\mu}$, i.e. matrix elements of the DC-symbol associated with Z'. In the oscillator limit we obtain a similar expression using (4.12) for the (n-2)-particle norm.

Note that the numbers $d'_{\bar{\mu},\mu}$ as well as the four numbers $\bar{\mu}(\bar{Z}(n-1))$, $\bar{\mu}(\bar{Z}(n))$, $\mu(Z''Z(n-1))$ and $\mu(Z''Z(n))$ are all we need to know about the permutations Z', Z'', $\bar{Z}$ and Z. Indeed these numbers characterize the double cosets generated by

these permutations according to References [8] and may be obtained directly without constructing the permutations.

5. Diastrophic and complex canonical transforms

In this section we shall discuss possibilities of a group theoretical interpretation of the method presented and we shall attempt a preliminary evaluation of the usefulness of such an interpretation.

These considerations are based on the quantum-mechanical representation of canonical transformations by Moshinsky and Quesne [21] and on diastrophic canonical transforms introduced by Klauder [22] and discussed for finite systems by Boiteux [23]. The use of the former in the present context was proposed in [24] and elaborated in [10, 12, 25, 26] while the use of the latter was proposed in [27].

We recall that according to [25] the linear canonical transformation in a $2m$ dimensional phase space

$$\begin{pmatrix} \bar{\mathbf{x}} \\ \bar{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{p} \end{pmatrix} \qquad \begin{aligned} ba^t &= ab^t \\ cd^t &= dc^t \\ da^t - cb^t &= I, \end{aligned} \tag{5.1}$$

where a, b, c, d are real $m \cdot m$ matrices, is represented by an integral operator with kernel

$$K(\bar{\mathbf{x}}, \mathbf{x}) = [(2\pi)^m |\det b|]^{-1/2} \exp\left\{\frac{i}{2}(\bar{\mathbf{x}}^t (b^t)^{-1} d^t \bar{\mathbf{x}} - 2\bar{\mathbf{x}}^t (b^t)^{-1}\mathbf{x} + \mathbf{x}^t a^t (b^t)^{-1}\mathbf{x})\right\} \tag{5.2}$$

if $\det b \neq 0$. If $\det b = 0$ the expression contains Dirac δ's and can be obtained by adequate limiting processes [25]. The representation is projective and thus we find that up to a phase, the product of two transformations will correspond to the folding of their respective kernels.

The canonical transformations (5.1) are a realization of the group $\mathcal{Sp}(2m, \mathbb{R})$ of real symplectic matrices and we may ask how the representation properties develop if we continue (5.2) to the group $\mathcal{Sp}(2m, \mathbb{C})$ corresponding to complex matrices a, b, c, d in (5.1). The answer is that the kernels do not represent this group but we have the so-called 'weak representation theorem' [26]. It states that, whenever the folding integral of two kernels exists (eventually in the sense of Dirac δ's) the resulting kernel corresponds to the product of the two matrices of $\mathcal{Sp}(2m, \mathbb{C})$ associated with the original kernels. The relation is established up to a phase by (5.2). A trivial consequence of this fact is that the subsemigroup of $\mathcal{Sp}(2m, \mathbb{C})$ corresponding to kernels of bounded operators is projectively represented by (3.2), [25], but such a restriction is not meaningful for our purposes. Comparing (5.2) with (2.12) we now find that $F(\mathbf{k}, \mathbf{x})$ corresponds to the matrix

$$\begin{pmatrix} iA^{-1} & -\frac{1}{2}I \\ I & -\frac{i}{2}A \end{pmatrix} \tag{5.3}$$

of $\mathcal{Sp}(2m, \mathbb{C})$ if I is an $m \cdot m$ unit matrix, i.e., is a complex extension of a Moshinsky–Quesne kernel. From the fact that the integral (2.5) does not converge for all values of $\gamma > 0$ we conclude that the corresponding operator is not bounded, but this causes no problem.

If we combine this result with the fact that several relevant two-body operators may either be given as complex canonical transforms (Gaussian interaction) or generated by such (kinetic energy) [25], it is easy to see that the integral (3.5) may be evaluated using the weak representation theorem. This was done in [10] for central interactions, the result being obviously identical to that obtained in Section 4 by completing squares. While the method is quite elegant for Gaussian interactions it becomes rather more involved for the kinetic energy, and extension to non-central interactions is possible but complicated, involving eventually inhomogeneous transforms. Advantages that may exist for angular momentum projection [26] seem also to be restricted to central interactions. The possibility of this interpretation ends at this point, because the proposal of reinterpreting the kernels for the cluster modes [10] is restricted to the case of equal numbers of clusters in bra and ket and presents certain problems even in this special case. This is too restrictive for nuclear reactions and it is obvious that we need transforms connecting spaces with different numbers of variables. In [27] it was proposed to use diastrophic canonical transforms [23] for this purpose. These are roughly speaking defined as follows:

Consider a set of canonical variables $\bar{x}_i, \bar{p}_i; i = 1 \ldots m$ that fulfil – as operators – the relation $[\bar{x}_i, \bar{p}_j]f = i\delta_{i,j}f, f \in D^m$, where D^m is a dense subset of $\mathcal{L}(\mathbb{R}^m)$ and another set $x_\alpha, p_\alpha; \alpha = 1 \ldots m + \mu$ with $[x_\alpha, p_\beta]F = i\,\delta_{\alpha,\beta}F$, $F \in D^{m+\mu}$ where $D^{m+\mu}$ is a dense subset of $\mathcal{L}(\mathbb{R}^{m+\mu})$. Then we call the transformation

$$\{\bar{x}_i, \bar{p}_i; i = 1 \ldots m\} \to \{x_\alpha, p_\alpha; \quad \alpha = 1 \ldots m + \mu\} \tag{5.4}$$

a diastrophic canonical transformation [23].

Boiteux [23] points out that a problem in m dimensions can be embedded into a problem with $m + \mu$ dimensions by such a transformation if we impose a superselection rule.

Apparently this type of idea may apply to kernels between different numbers of clusters but more important it applies to the process of freezing internal coordinates as it was pointed out in [27]. Indeed we could start by assuming that the resonating group wave function actually describes our system which interacts by complicated non-local potentials. By extending our space from κ to n variables we would then obtain a local description in these n variables with the additional restrictions that the internal functions of certain substructures are fixed. This restriction plays the role of a superselection rule. Actually the situation is reversed because we have an n nucleon system and wish to restrict it to a κ-cluster system. The approximation involved then appears as the imposition of a superselection rule that is only approximately valid. Coupling kernels between different cluster structure are correction terms that appear if we allow alternatively two or more superselection rules.

Practically the theory of diastrophic canonical transforms is not sufficiently well worked out at present to give a definitive answer to the question whether further simplifications of the results obtained by pedestrian methods in Sections 3 and 4 are possible, but it is very doubtful that any advantage of this type may be gained. On the other hand we see that diastrophic transformations are intimately related to the very ideas of the resonating group method and in distinction to complex canonical transforms they do shed a new light into the concept of clustering as an approximative

superselection principle. Note that the principle is quite general and need not relate to free clusters. Distortions etc. may be taken into account and the notion of competing approximative superselection rules for different cluster structures is very suggestive. It therefore seems worth while to investigate this approach further as soon as more knowledge about diastrophic canonical transformations is available.

Appendix

In this appendix we shall give explicit expressions for the two-body kernels H'' of equation (4.8) resulting from the most important two-body operators.

In order to avoid unnecessarily complicated indices we make the replacements of variables:

$$\begin{aligned}
&\vec{x}^{n-1} \to \vec{y}^1; \qquad \vec{x}^n \to \vec{y}^2 \\
&\vec{k}^{Z''Z(n-1)} \to \vec{q}^1; \qquad \vec{k}^{Z''Z(n)} \to \vec{q}^2 \\
&\vec{\bar{k}}^{\bar{Z}(n-1)} \to \vec{\bar{q}}^1; \qquad \vec{\bar{k}}^{\bar{Z}(n)} \to \vec{\bar{q}}^2 \\
&\alpha_{Z''Z(n-1)} \to \beta_1; \qquad \alpha_{Z''Z(n)} \to \beta_2 \\
&\bar{\alpha}_{\bar{Z}(n-1)} \to \bar{\beta}_2; \qquad \bar{\alpha}_{\bar{Z}(n)} \to \bar{\beta}_2.
\end{aligned} \tag{A.1}$$

We shall deal with the following two-body operators:

(*a*) *Central potential*

$$\mathcal{T}_c(1,2) = \exp\{-\tfrac{1}{2}\Gamma_c(\vec{y}^1 - \vec{y}^2)^2\} \tag{A.2}$$

(*b*) *Spin-orbit potential*

$$\mathcal{T}_{so}(1,2) = \exp\{-\tfrac{1}{2}\Gamma_{so}(\vec{y}^1 - \vec{y}^2)^2\} \frac{\hbar}{i}(\vec{y}^1 - \vec{y}^2) \times (\vec{\nabla}^1 - \vec{\nabla}^2) \tag{A.3}$$

(*c*) *Tensor potential*

$$\mathcal{T}_t(1,2) = \exp\{-\tfrac{1}{2}\Gamma_t(\vec{y}^1 - \vec{y}^2)^2\} (\vec{y}^1 - \vec{y}^2)^2 \, Y_{2m}(\Omega_{(\vec{y}^1 - \vec{y}^2)}) \tag{A.4}$$

(*d*) *Kinetic energy*

$$\mathcal{T}_k(1,2) = \left(-\frac{\hbar^2}{2m}\right)(\vec{\nabla}^1 - \vec{\nabla}^2)^2 \tag{A.5}$$

In order to include the possibility of approximative treatment of Jastrow factors [20] we will actually allow two-body operators of the form

$$T_{(1,2)} = \exp\{-\tfrac{1}{2}\Gamma_l(\vec{y}^1 - \vec{y}^2)^2\} \mathcal{T}(1,2) \exp\{-\tfrac{1}{2}\Gamma_r(\vec{y}^1 - \vec{y}^2)^2\} \tag{A.6}$$

The results for the standard operators $\mathcal{T}(1, 2)$ are somewhat simpler and may be retrieved by setting $\Gamma_l = \Gamma_r = 0$.

In order to treat the tensor potential it proves useful to consider the generating function [28]

$$\exp\{ia(\vec{\Lambda}(b)\cdot\vec{r})\} = \exp\{a[r_1 + ir_2 - 2r_3 b - (r_1 - ir_2)b^2]\}$$
$$= \sum_{L=0}^{\infty} \frac{(ia)^L b^L r^L}{L!} \sum_{m=-L}^{L} \left(\frac{4\pi}{2L+1}\cdot\frac{1}{(L-m)!(L+m)!}\right)^{1/2} b^{-m} Y_{Lm}(\Omega_{\vec{r}}) \quad \text{(A.7)}$$

of solid harmonics which will also be used with advantage to integrate over the coordinates of relative motion of the clusters, that may carry angular momentum [3].

To present the final results in compact form we shall use the abbreviations

(a) $\Gamma = \Gamma_l + \Gamma_c + \Gamma_r$ (central potential)
(b) $\Gamma = \Gamma_l + \Gamma_{so} + \Gamma_r$ (spin-orbit potential)
(c) $\Gamma = \Gamma_l + \Gamma_t + \Gamma_r$ (tensor potential)
(d) $\Gamma = \Gamma_l + \Gamma_r$ (kinetic energy)

as well as

$$\zeta_1 = \bar{\alpha}_1 + \alpha_1 + \Gamma$$
$$\zeta_2 = \bar{\alpha}_2 + \alpha_2 + \Gamma \quad \text{(A.8)}$$

and finally

$$I_0 = (2/\pi)^3(\zeta_1\zeta_2 - \Gamma^2)^{-3/2}$$
$$\exp\left\{-\frac{2}{\zeta_1\zeta_2 - \Gamma^2}[\zeta_2(\vec{\bar{q}}^1 - \vec{q}^1)^2 + 2\Gamma(\vec{\bar{q}}^1 - \vec{q}^1)\cdot(\vec{\bar{q}}^2 - \vec{q}^2)\right.$$
$$\left. + \zeta_1(\vec{\bar{q}}^2 - \vec{q}^2)^2]\right\}$$
$$\exp\left\{\frac{1}{\bar{\alpha}_1}(\vec{\bar{q}}^1)^2 + \frac{1}{\bar{\alpha}_2}(\vec{\bar{q}}^2)^2 + \frac{1}{\alpha_1}(\vec{q}^1)^2 + \frac{1}{\alpha_2}(\vec{q}^2)^2\right\}. \quad \text{(A.9)}$$

We can now give the two-body kernels

$$H''(\vec{\bar{q}}^1, \vec{\bar{q}}^2; \vec{q}^1, \vec{q}^2) = \pi^{-6} \int\int d\vec{y}^1\, d\vec{y}^2$$
$$\left(\prod_{s=1}^{2} \exp\left\{-\frac{1}{2}\bar{\alpha}_s(\vec{y}^s)^2 - 2i\vec{y}^s\cdot\vec{\bar{q}}^s + \frac{1}{\bar{\alpha}_s}(\vec{\bar{q}}^s)^2\right\}\right)$$
$$T_{(1,2)}\left(\prod_{s=1}^{2} \exp\left\{-\frac{1}{2}\alpha_s(\vec{y}^s)^2 + 2i\vec{y}^s\cdot\vec{q}^s + \frac{1}{\alpha_s}(\vec{q}^s)^2\right\}\right) \quad \text{(A.10)}$$

explicitly for the different two-body operators:

(*a*) *Central potential*

$$H''(\vec{\bar{q}}^1, \vec{\bar{q}}^2; \vec{q}^1, \vec{q}^2) = I_0 \quad \text{(A.11)}$$

(*b*) *Spin-orbit potential*

$$H''(\bar{\vec{q}}^1, \bar{\vec{q}}^2; \vec{q}^1, \vec{q}^2) = 4i\hbar \frac{1}{\zeta_1\zeta_2 - \Gamma^2} I_0 \cdot \{[(\bar{\alpha}_2 + \alpha_2)(\bar{\vec{q}}^1 - \vec{q}^1) - (\bar{\alpha}_1 + \alpha_1)(\bar{\vec{q}}^2 - \vec{q}^2)] \times (\vec{q}^2 - \vec{q}^1) - (\alpha_1 - \alpha_2)(\bar{\vec{q}}^1 - \vec{q}^1) \times (\bar{\vec{q}}^2 - \vec{q}^2)\} \quad \text{(A.12)}$$

(*c*) *Tensor potential*

$$H''(\bar{\vec{q}}^1, \bar{\vec{q}}^2; \vec{q}^1, \vec{q}^2) = I_0 \exp\left\{-\frac{2a}{\zeta_1\zeta_2 - \Gamma^2} \vec{\Lambda}(b) \cdot [(\bar{\alpha}_1 + \alpha_1)(\bar{\vec{q}}^2 - \vec{q}^2) - (\bar{\alpha}_2 + \alpha_2)(\bar{\vec{q}}^1 - \vec{q}^1)]\right\} \quad \text{(A.13)}$$

(*d*) *Kinetic energy*

$$H''(\bar{\vec{q}}^1, \bar{\vec{q}}^2; \vec{q}^1, \vec{q}^2) = \frac{\hbar^2}{2M} I_0 \cdot \left[3\left\{(\alpha_1 + \alpha_2 + 4\Gamma_r) - \frac{1}{\zeta_1\zeta_2 - \Gamma^2}\left[\zeta_2(\alpha_1 + 2\Gamma_r)^2 - 2\Gamma(\alpha_1 + 2\Gamma_r)(\alpha_2 + 2\Gamma_r) + \zeta_1(\alpha_2 + 2\Gamma_r)^2\right]\right\} + 4\left\{(\vec{q}^2 - \vec{q}^1) + \frac{1}{\zeta_1\zeta_2 - \Gamma^2}[(\zeta_2(\alpha_1 + 2\Gamma_r) - \Gamma(\alpha_2 + 2\Gamma_r)) \cdot (\bar{\vec{q}}^1 - \vec{q}^1) - (\zeta_1(\alpha_2 + 2\Gamma_r) - \Gamma(\alpha_1 + 2\Gamma_r))(\bar{\vec{q}}^2 - \vec{q}^2)]\right\}^2\right]. \quad \text{(A.14)}$$

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