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Systematic analysis of integral kernels in generator coordinate theories for nucleus-nucleus scattering

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The structure of generator coordinate kernels for nucleus-nucleus scattering is analyzed with respect to various particle exchange contributions due to antisymmetrization. This analysis leads to an algorithm for a systematic computation of the kernels, and is suitable for revealing their analytical form. The method may be used as a guideline for computer aided symbolic algebra calculations.

[NUCLEAR REACTIONS Classification of GC integral kernels with respect to particle exchange. Systematic computation.]

I. INTRODUCTION

Generator coordinate (GC) theories have become a powerful tool for microscopic investigations in nucleus-nucleus scattering. Typically, the scattering system is described by Slater determinants (or superpositions of Slater determinants) which represent two (or more) clusters with their relative degrees of freedom being parametrized by real or complex generator coordinates. The most direct application of these techniques is the generator coordinate method (GCM) (Refs. 1–3) where the Hill-Wheeler equations[4] have to be solved directly with appropriate boundary conditions. Generator coordinate techniques also seem to be indispensable when performing resonating group method (RGM) (Refs. 5 and 6) calculations for heavier systems. The integral kernels in the RGM may either be obtained by unfolding the corresponding GCM kernels[7–9] or by introducing complex generator coordinates (CGCM) (Refs. 10, 6, and 11) and integrating over some of these. All these techniques depend crucially on the factorization of the center-of-mass motion in each cluster Slater state and therefore demand describing the individual nuclei in the scattering system by harmonic oscillator model wave functions. During the past decade dynamical scattering calculations within microscopic theories have been performed persistently with harmonic oscillator models. Much has been learned within this framework (and still is) although the description of the individual nuclei appears to be poor as far as the nuclear structure is concerned.

It appears desirable to treat inelastic processes in a microscopic fashion. Nuclear reactions can be calculated within the coupled channel framework, again, with each fragment being in a harmonic oscillator ground state.[12] The alternative approach of an inelastic scattering process where one of two partners can undergo an internal excitation turns out to be troublesome even within an oscillator model because the center-of-mass motion does not factorize in general[13] and thus there is no longer an easy way to restore translational invariance.

The possibility of treating more general wave functions than "Gaussians multiplied by polynomials" is, however, desirable and will be stimulating to microscopic nucleus-nucleus scattering theories. For example, inelastic processes which lead to excitations of one nucleus in the continuous energy spectrum may be investigated by including single particle states with "plane wave boundary conditions" in the Slater determinant model states.[14] In this and other similar cases a reasonable form of translational invariant two-fragment states is

$$\mathscr{A}_{12}\{(2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{x}_{\rm rel})\phi^{(1)}_{{\rm int},n_1}(\xi_1)\phi^{(2)}_{{\rm int},n_2}(\xi_2)\}\ , \tag{1.1}$$

where $\vec{x}_{\rm rel}$ and ξ_1,ξ_2 are the relative and internal coordinates, respectively. $\mathscr{A}_{12}$ is the antisymmetrizer between the two nuclei, and the subscripts n_1 and n_2 on the internal wave functions $\phi^{(i)}_{{\rm int},n_i}$, $i=1,2$, denote excitations built into the one-fragment model states. Using a generator coordinate approach in order to calculate overlap and Hamiltoni-

an matrix elements with the states (1.1) one usually starts out with (noninvariant) one-fragment Slater states which are displaced in coordinate and (in general) in momentum space by, say, $\vec{r}_i$ and $\vec{k}_i$, respectively. Let us write these states as

$$C^{\dagger}_{i,n_i}(\vec{r}_i,\vec{k}_i)\,|\,0\rangle\ ,\quad i=1,2\ ,$$

using creation operators acting on the vacuum $|\,0\rangle$. Rather than by "mathematical accident" like in oscillator models, translational (and Galilean) invariance must then be restored by more elaborate methods as, e.g., projection operator techniques. This apparently leads to an increase of calculational and numerical effort which one must be able to cope with efficiently. To illustrate this point, which this work is (partly) devoted to, we quote that an application of the Rouhaninejad-Yoccoz projection method[15] allows us to compute matrix elements with the states (1.1) out of generator coordinate integral kernels by means of the integral transformation[16,14]

$$\langle\bar{\phi}(\vec{k}'n')\,|\,K_{\rm op}\,|\,\bar{\phi}(\vec{k}n)\rangle_{\rm INT}$$
$$=\int d^3s_1\int d^3s_2\int d^3u\exp\left[-\frac{i}{2}(\vec{k}'+\vec{k})\cdot(\vec{s}_1-\vec{s}_2)-i(\vec{k}'-\vec{k})\cdot\vec{u}\right]K_{n'n}(\vec{s}_1\vec{s}_2\vec{u};\vec{k}'\vec{k})\ , \tag{1.2a}$$

$$K_{n'n}(\vec{s}_1\vec{s}_2\vec{u};\vec{k}'\vec{k})=\left\langle 0\left|C_{1n'_1}\left[-\frac{\vec{s}_1}{2}-\frac{N_2}{N}\vec{u},-\vec{k}'\right]C_{2n'_2}\left[-\frac{\vec{s}_2}{2}+\frac{N_1}{N}\vec{u},\vec{k}'\right]\right.\right.$$
$$\left.\left.\times K_{\rm op}C^{\dagger}_{2n_2}\left[\frac{\vec{s}_2}{2}+\frac{N_1}{N}\vec{u},\vec{k}\right]C^{\dagger}_{1n_1}\left[\frac{\vec{s}_1}{2}-\frac{N_2}{N}\vec{u},-\vec{k}\right]\right|0\right\rangle\ , \tag{1.2b}$$

where $K=1$ or $K=H$, $|\,\bar{\phi}(\vec{k}n)\rangle$ denotes the translational invariant states (1.1), and N_1,N_2, and $N=N_1+N_2$ are the mass numbers in the system. Note that the matrix element on the left hand side of Eq. (1.2a) is meant with respect to the internal variables ξ_1, ξ_2, and $\vec{x}_{\rm rel}$, as indicated by the subscript INT, whereas the right hand side of Eq. (1.2b) is a usual GC matrix element defined with respect to all single particle coordinates $\vec{x}_1,\ldots,\vec{x}_N$; it plays the role of a GC integral kernel. This kernel is accessible by standard determinantal methods[17,18] (Wick's theorem), however, it depends on five vector variables; three of these have to be integrated over in a Fourier-type integral, Eq. (1.2a). Although this appears to be impracticable at a first sight it is, nevertheless, relatively straightforward (and has been done in practice in the work of Ref. 14) to apply the transformation formulas (1.2) provided the following prerequisites are met:

(i) the structure of the GC kernel $K_{n'n}(\vec{s}_1\vec{s}_2\vec{u};\vec{k}'\vec{k})$ is analytically known,

(ii) symbolic algebra computer codes can be employed to perform the three Fourier-integrals in (1.2a).

Requirement (i) can be fulfilled in oscillator models (with equal or unequal widths) and Gaussian nucleon-nucleon forces.[19] (The Coulomb force may also be treated by a sum of Gaussians.[20]) However, we emphasize that one may equally well use, e.g., plane wave single particle states (or the Fourier representation of an arbitrary state) in order to describe excited nuclei. The center-of-mass motion is automatically treated correctly if the momentum projection technique, i.e., essentially Eqs. (1.2) is used.[16] In either case the *compact* determinantal structure of the GC kernels, as provided by the formulas of Löwdin and Brink,[17,18] cannot be maintained; a detailed analysis of the GC kernels with respect to their analytical structure is necessary in order to make a symbolic algebra[21] integration possible. It may even be necessary to perform a

(iii) computer aided calculation of the analytic form of the GC kernels,

where one starts out with one-body and two-body single particle matrix elements.

In the present paper we propose a systematic way for calculating the overlap, one-body, and two-body GC integral kernels decomposed into parts of distinct analytical structure. A particularly important feature of the method is that the symmetries of the system (e.g., rotational invariance) are utilized at a very early stage and are preserved in each intermediate step of the calculation. This comes about because invariant expressions are generated by performing traces which involve one- (two-) particle matrix elements. Since, in this way, the symmetries become manifest, the analytic functions one has to deal with depend only on a limited number of invariant combinations of the generator coordinates.

Apart from this technical aspect the algorithm

described here exhibits the

(iv) structure of the kernels with respect to particle exchange between the fragments

and, within each subkernel with the same number of particles exchanged it is still possible to distinguish

(v) various classes of contributions to the Hamiltonian kernels due to different exchange processes, each of which is consistent with the symmetry properties of the system.

At the present, rather progressed, state of generator coordinate techniques,[22,23] it is not surprising that symbolic algebra computer codes have already been applied in microscopic calculations of nucleus-nucleus scattering.[19,24] There also have been attempts to classify GC integral kernels with respect to particle exchange.[19,25] However, all this work has been done within the constraint of harmonic oscillator models. This is also true for the detailed particle-exchange classification schemes developed in Ref. 19. The results there are, in principle, reproduced by specializing the more general algorithm proposed in the present work. It should also be mentioned that the formulas (1.2) which originate from a momentum projection approach only serve as an example to illustrate the complexity of the calculational problems. The algorithm developed in the following sections is more general.

We will first treat the overlap kernel (Sec. II) and then extend the method to GC kernels involving one-particle operators (e.g., kinetic energy, Sec. III) and two-particle operators (potential energy, Sec. IV). The resulting formulas can be simplified further by utilizing the orthogonality of spin-isospin states; as an example we will treat the case of $4N$-nuclear states in Sec. VI.

The present algorithm has already been applied to the calculation of integral kernels using formulas (1.2) (and symbolic computer algebra) in the case of α-α scattering[14]; the model considered there includes excitations of an α particle to the continuous energy spectrum and thus goes beyond the harmonic oscillator framework.

II. THE NORM KERNEL

We consider model states to two-center Slater determinants that carry a set of generator coordinates q which are grouped into two subsets, q_1 and q_2, each parametrizing the center-of-mass degrees of freedom of the nuclei with particle numbers N_1 and N_2. q_1 may be the mean position, the mean momentum, or some more sophisticated, e.g., complex, parameter associated with nucleus I, $I=1,2$. The norm kernel $\mathcal{N}(q',q)$, i.e., the overlap of the corresponding Slater states, can be written as the determinant of the $N\times N$ overlap matrix[17,18] $M(q',q)$,

$$\mathcal{N}(q',q)=\det M(q',q)\ . \tag{2.1}$$

The matrix $M(q',q)$ is composed of four block matrices,

$$M(q',q)=\begin{bmatrix} M^{11}(q_1',q_1) & M^{12}(q_1',q_2) \\ M^{21}(q_2',q_1) & M^{22}(q_2',q_2) \end{bmatrix}, \tag{2.2}$$

provided that the fragmentation $N=N_1+N_2$ is the same on both bra and ket sides. However, the set of the one particle states, which determine the matrices $M^{IJ}(q_I',q_J)$, $I,J=1,2$, i.e.,

$$M_{ij}^{IJ}(q_I'q_J)=\int dx\ \phi_i^I(x,q_I')^\dagger\psi_j^J(x,q_J)\ , \tag{2.3}$$

may be chosen differently on either side.

We now assume that $\det M^{11}$ and $\det M^{22}$ are not identical to zero and have, as functions of the generator coordinates, at most discrete zero points. For example, in GCM approaches to elastic scattering of nuclei in their ground state, described by an oscillator shell model, $\det M^{II}$ is simply a Gaussian and therefore is nonzero for arbitrary values of q_I' and q_I. The assumption may also be true for a considerably wide class of kernels describing transitions to channels with excited fragments.[26] For all generator coordinates where $\det M^{11}\neq 0$ and $\det M^{22}\neq 0$ it is thus legitimate to define

$$\begin{aligned} \omega^{12}&=(M^{11})^{-1}M^{12}\ , \\ \omega^{21}&=(M^{22})^{-1}M^{21}\ , \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} \Omega^{11}&=\omega^{12}\omega^{21}\ , \\ \Omega^{22}&=\omega^{21}\omega^{12}\ . \end{aligned} \tag{2.5}$$

Thus the overlap matrix M can be written as a fourfold product

$$M=\begin{bmatrix} M^{11} & 0 \\ 0 & M^{22} \end{bmatrix}\begin{bmatrix} 1 & \omega^{12} \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1-\Omega^{11} & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ \omega^{21} & 1 \end{bmatrix}, \tag{2.6a}$$

or alternatively,

$$M=\begin{bmatrix} M^{11} & 0 \\ 0 & M^{22} \end{bmatrix}\begin{bmatrix} 1 & 0 \\ \omega^{21} & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1-\Omega^{22} \end{bmatrix}\begin{bmatrix} 1 & \omega^{12} \\ 0 & 1 \end{bmatrix}. \tag{2.6b}$$

Then the norm kernel reads

$$\mathcal{N}=\det M^{11}\det M^{22}\det(1-\Omega^{11})\,, \tag{2.7a}$$

$$\mathcal{N}=\det M^{11}\det M^{22}\det(1-\Omega^{22})\,. \tag{2.7b}$$

A determinant of type $\det(1-\lambda\Omega)$, with an $n\times n$ matrix Ω and λ being a parameter, can be expanded in powers of λ,[27,28]

$$\det(1-\lambda\Omega)=\sum_{\nu=0}^{n}\lambda^{\nu}\Delta_{\nu}\,. \tag{2.8}$$

The expansion coefficients are

$$\Delta_{\nu}=\frac{1}{\nu!}\left[\left[\frac{d}{d\lambda}\right]^{\nu}\det(1-\lambda\Omega)\right]_{\lambda=0}$$
$$=\frac{(-)^{\nu}}{\nu!}\sum_{k_1=1}^{n}\cdots\sum_{k_\nu=1}^{n}\det\begin{bmatrix}\Omega_{k_1k_1} & \cdots & \Omega_{k_1k_\nu}\\ \vdots & & \vdots\\ \Omega_{k_\nu k_1} & \cdots & \Omega_{k_\nu k_\nu}\end{bmatrix}. \tag{2.9}$$

This treatment of $\det(1-\lambda\Omega)$ is, so far, analogous to the Fredholm method (cf. Sec. 9.3 in Ref. 29).

We now write the $\nu\times\nu$ determinants in (2.9) explicitly as

$$\det(\Omega_{k_ik_j})=\sum_{\pi\in s_\nu}(-)^{\pi}\Omega_{k_1\pi(k_1)}\cdots\Omega_{k_\nu\pi(k_\nu)} \tag{2.10}$$

(with s_ν being the permutation group of ν elements) and then decompose each π into an irreducible product of cycles

$$\pi=\underbrace{(\,)_1\cdots(\,)_1}_{m_1}\cdots\underbrace{(\,)_l\cdots(\,)_l}_{m_l}\cdots\underbrace{(\,)_\nu\cdots(\,)_\nu}_{m_\nu}\,.$$

Here the multiplicities m_l—i.e., the number of (different) cycles $(\,)_l$ with common length l—are subject to the condition[30]

$$\sum_{l=1}^{\nu}lm_l=\nu,\quad m_l\geq 0\,. \tag{2.11}$$

Inserting (2.10) into (2.9) the ν-fold product of the Ω-matrix elements can be reordered as indicated by the cycles. Accordingly the summations in (2.9) are written as m_l-fold products of subsummations within the respective cycles and thus lead to traces of powers of Ω. We therefore define

$$\Gamma_l=\mathrm{tr}\Omega^{l} \tag{2.12}$$

and obtain

$$\sum_{k_1=1}^{n}\cdots\sum_{k_\nu=1}^{n}\Omega_{k_1\pi(k_1)}\cdots\Omega_{k_\nu\pi(k_\nu)}=\Gamma_1^{m_1}\cdots\Gamma_\nu^{m_\nu}\,.$$

Since the number of permutations characterized by an array $(m_1\cdots m_\nu)$ is given by[30]

$$\frac{\nu!}{m_1!1^{m_1}\cdots m_\nu!\nu^{m_\nu}}$$

and since the relation

$$(-)^{\pi}=(-1)^{\nu+m_1+\cdots+m_\nu}$$

holds, we obtain the result

$$\Delta_{\nu}=\sum_{(m_1\cdots m_\nu)}\frac{(-1)^{m_1+\cdots+m_\nu}}{m_1!1^{m_1}\cdots m_\nu!\nu^{m_\nu}}\Gamma_1^{m_1}\cdots\Gamma_\nu^{m_\nu}\,. \tag{2.13}$$

The sum comprises all arrays $(m_1\cdots m_\nu)$ that satisfy condition (2.11).

We now include a factor $\sqrt{\lambda}$ in both ω^{12} and ω^{21} and then identify Ω with Ω^{II} and n with N_I, I being 1 or 2. Thus it can be concluded from (2.7a), (2.7b), and (2.8) that the relation

$$\sum_{\nu=0}^{N_1}\lambda^{\nu}\Delta_{\nu}^{(1)}=\sum_{\nu=0}^{N_2}\lambda^{\nu}\Delta_{\nu}^{(2)} \tag{2.14}$$

holds, where $\Delta_\nu^{(1)}$ and $\Delta_\nu^{(2)}$ correspond to Ω^{11} and Ω^{22}, respectively. Since the expansion coefficients on either side must be the same, the norm kernel reads

$$\mathcal{N}=\sum_{\nu=0}^{\min(N_1,N_2)}\mathcal{N}_{\nu}\,, \tag{2.15a}$$

$$\mathcal{N}_{\nu}=\det M^{11}\det M^{22}\Delta_{\nu}\,. \tag{2.15b}$$

Here Δ_ν is defined by (2.13) and (2.12) while it makes no difference if Ω is chosen to be Ω^{11} or Ω^{22}; one may conveniently choose the matrix of smaller size.

There are some significant features of our result that are worth mentioning:

(a) The prescription for calculating the norm kernel is most suitable for calculations on a computer. The powers of the matrix Ω as well as the contributions to (2.13) may be computed in a *recursive* manner.

(b) The invariance properties of the model states with respect to transformations under a certain symmetry group are manifestly preserved when performing the trace in (2.12). Symmetry properties, which normally help to reduce numerical effort, can thus be utilized at a very early stage of computation.

(c) The terms in the decomposition (2.14) admit a simple interpretation. Since the matrix elements of $M^{IJ}(q_I',q_J)$ are (non-normalized) transition ampli-

tudes from "ket J" to "bra I," one may associate a one-particle exchange process with the matrix

$$\Omega^{11}=(M^{11})^{-1}M^{12}(M^{22})^{-1}M^{21}\ ,$$

or alternatively, with

$$\Omega^{22}=(M^{22})^{-1}M^{21}(M^{11})^{-1}M^{12}\ .$$

We therefore interpret $\mathcal{N}_\nu$ as the ν-particle exchange contribution to the norm kernel. In Eq. (2.13) all possible ways to exchange ν nucleons between the fragments are taken into account.

The norm kernel contribution $\mathcal{N}_\nu$ may be illustrated graphically: Since, for each ν, the $m_\nu=1$ term in Eq. (2.13) can be uniquely attached to $\mathcal{N}_\nu$,

$$\mathcal{N}_\nu=\det M^{11}\det M^{22}(-\Gamma_\nu/\nu)+\cdots\ ,$$

it is sufficient to visualize Γ_ν. For example, Fig. 1 represents $\mathcal{N}_1$, where the characteristic trace is

$$\Gamma_1=\mathrm{tr}[(M^{22})^{-1}M^{21}(M^{11})^{-1}M^{12}]\ .$$

The boxes denote the fragments in the bra and ket states, respectively; the dotted and solid lines represent $(M^{11})^{-1}$, $(M^{22})^{-1}$, and M^{12},M^{21}, respectively. Performing the trace is indicated by *closing* the lines. This picture may be generalized in an obvious manner to $\nu>1$, i.e., to the illustration of the terms $\Gamma_1^{m_1}\cdots\Gamma_\nu^{m_\nu}$ with $m_\nu>1$ by drawing several closed loops where each loop is identified with the corresponding trace Γ_l.

III. THE KINETIC ENERGY KERNEL

The generator coordinate kernel $\mathcal{T}$ of a one-body operator, say the kinetic energy, can be calculated and classified on the same footing as the norm kernel.

We start from the general form[18]

$$\mathcal{T}=\mathrm{tr}[c_1^t(M)t]\ , \tag{3.1}$$

where $c_1^t(M)$ is the transposed first order cofactor matrix of M, cf. (2.2), and t denotes the matrix of the one-particle operator t_{op} which, again, is written in block form,

$$t=\begin{bmatrix} t^{11} & t^{12} \\ t^{21} & t^{22} \end{bmatrix}\ , \tag{3.2}$$

$$t_{ij}^{IJ}(q_I'q_J)=\int dx\phi_i^I(x,q_I')^\dagger t_{\mathrm{op}}(x)\psi_j^J(x,q_J)\ . \tag{3.3}$$

In order to evaluate $c_1^t(M)$ the relations

$$c_1(PQ)=c_1(P)c_1(Q) \tag{3.4}$$

and

$$c_1^t(P)=P^{-1}\det P,\quad \det P\neq 0\ , \tag{3.5}$$

are applied to both Eqs. (2.6a) and (2.6b). By comparing the two results one obtains

$$c_1^t(M)=\begin{bmatrix} c_1^t(1-\Omega^{11}) & -c_1^t(1-\Omega^{11})\omega^{12} \\ -\omega^{21}c_1^t(1-\Omega^{11}) & c_1^t(1-\Omega^{22}) \end{bmatrix} \times\begin{bmatrix} (M^{11})^{-1} & 0 \\ 0 & (M^{22})^{-1} \end{bmatrix}\det M^{11}\det M^{22}\ . \tag{3.6}$$

We note that deriving (3.6) in this way leads to

$$c_1^t(1-\lambda\Omega^{11})=1\det(1-\lambda\Omega^{22}) +\lambda\omega^{12}c_1^t(1-\lambda\Omega^{22})\omega^{21}\ , \tag{3.7a}$$

$$c_1^t(1-\lambda\Omega^{11})\omega^{12}=\omega^{12}c_1^t(1-\lambda\Omega^{22})\ , \tag{3.7b}$$

and two additional relations obtained from (3.7a) and (3.7b) by simply interchanging the upper indices 1 and 2. Thus we are left with the problem of calculating cofactors of a matrix $(1-\lambda\Omega)$; these are expanded in powers of λ,

$$c_1^t(1-\lambda\Omega)=\sum_{\nu=0}^{n-1}\lambda^\nu X_\nu\ . \tag{3.8a}$$

Inserting this into

$$(1-\lambda\Omega)c_1^t(1-\lambda\Omega)=1\det(1-\lambda\Omega)$$

and using (2.8) we obtain the recursion formulas

$$X_0=1\ ,$$

$$X_\nu=1\Delta_\nu+X_{\nu-1}\Omega,\quad 1\le\nu\le n-1\ ,$$

$$0=1\Delta_n+X_{n-1}\Omega\ .$$

By induction, one concludes that

$$X_\nu=\sum_{\mu=0}^{\nu}\Delta_{\nu-\mu}\Omega^\mu\ . \tag{3.8b}$$

Now inserting (3.6) into (3.1) and using Eqs. (3.8) yields the final result

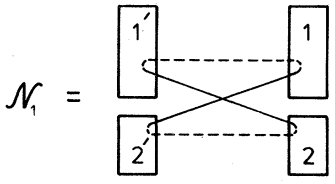

FIG. 1. Graphical illustration of the one particle exchange contribution to the norm kernel.

$$\mathcal{T}=\sum_{IJ}\sum_{\nu=0}^{m[IJ]}\mathcal{T}_\nu^{IJ}\ , \tag{3.9a}$$

$$\mathcal{T}_\nu^{IJ}=\det M^{11}\det M^{22}\sum_{\mu=0}^{\nu}\Delta_{\nu-\mu}\theta_\mu^{IJ}\ . \tag{3.9b}$$

The traces θ_μ^{IJ}, which include the matrix elements of the one-particle operator, are listed in Table I, where the abbreviations

$$T^{IJ}=(M^{II})^{-1}t^{IJ},\quad I,J=1,2 \tag{3.10}$$

are used. The boundaries $m[IJ]$, which are also listed in Table I, result from comparing the degrees of the λ polynomials on both sides of Eqs. (3.7). In the last column of the table one finds the number of particles exchanged between the fragments, which has to be attached to the contribution $\mathcal{T}_\nu^{IJ}$. In analogy to Sec. II $\mathcal{T}_\nu{}^{11}$ and $\mathcal{T}_\nu{}^{22}$ represent ν-particle exchange terms, whereas $\mathcal{T}_\nu{}^{12}$ and $\mathcal{T}_\nu{}^{21}$ are $(\nu+1)$-particle exchange contributions because the matrices $T^{12}\omega^{21}$ and $\omega^{12}T^{21}$ describe an additional particle exchange process via the matrix elements of the one-particle operator. This feature is visible in the graphics of Fig. 2, where the kernels $\mathcal{T}_\nu^{IJ}$, $\nu=0$, are illustrated. Here the cross represents the one-particle operator.

IV. THE INTERACTION KERNEL

In order to treat a generator coordinate kernel $\mathcal{V}$ of a two-body operator $v_{\rm op}$, say the potential energy, in a similar manner we start from[18]

$$\begin{aligned}\mathcal{V}&=\tfrac{1}{2}\mathrm{tr}[c_2^t(M)v]\\ &:=\tfrac{1}{2}\sum_{\alpha\beta}\sum_{\gamma\delta}c_2^t(M)_{\gamma\delta,\alpha\beta}v_{\alpha\beta,\gamma\delta}\ ,\end{aligned} \tag{4.1}$$

where tr here denotes a "tensor trace." The two-particle matrix elements $v_{\alpha\beta,\gamma\delta}$ are written in block form

$$v_{ij}^{IJ,KL}(q_I'q_J',q_Kq_L)=\int dx_1\int dx_2\phi_i^I(x_1,q_I')^\dagger\phi_j^J(x_2,q_J')^\dagger v_{\rm op}(1,2)\psi_k^K(x_1,q_K)\psi_l^L(x_2,q_L)\ , \tag{4.2}$$

with the identification $\alpha=(I,i),\ldots,\delta=(L,l)$, and $c_2^t(M)$ denoting the transposed second order cofactor tensor of M. Analogous to (3.4) and (3.5) the relations

$$c_2(PQ)=\tfrac{1}{2}c_2(P)c_2(Q) \tag{4.3}$$

and

$$c_2^t(P)=P^{-1}\times P^{-1}\det P,\quad \det P\neq 0\ , \tag{4.4}$$

hold [tensor multiplications as in (4.1)]; here we have defined

$$(P\times Q)_{\alpha\beta,\gamma\delta}=P_{\alpha\gamma}Q_{\beta\delta}-P_{\alpha\delta}Q_{\beta\gamma} \tag{4.5}$$

for two matrices P and Q. Tensors of this type have the property

$$(P\times Q)(R\times S)=PR\times QS+PS\times QR\ . \tag{4.6}$$

When applying (4.3) and (4.4) to the decompositions (2.6a) and (2.6b) it turns out that the second order cofactor tensor of a matrix $(1-\lambda\Omega)$ has to be calculated. A straightforward calculation yields a result that is formally similar to (3.8)

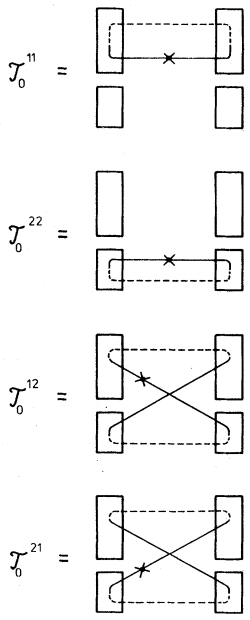

FIG. 2. Graphical illustration of the simplest contributions to the kinetic energy kernel.

TABLE I. Traces involving one-particle operators.

IJ	θ_μ^{IJ}	min$[IJ]$	
11	$\mathrm{tr}[(\Omega^{11})^\mu T^{11}]$	$\min(N_1-1,N_2)$	ν
22	$\mathrm{tr}[(\Omega^{22})^\mu T^{22}]$	$\min(N_1,N_2-1)$	ν
12	$-\mathrm{tr}[\omega^{21}(\Omega^{11})^\mu T^{12}]$	$\min(N_1-1,N_2-1)$	$\nu+1$
21	$-\mathrm{tr}[(\Omega^{11})^\mu\omega^{12}T^{21}]$	$\min(N_1-1,N_2-1)$	$\nu+1$

$$c_2^t(1-\lambda\Omega)=\sum_{\nu=0}^{n-2}\lambda^\nu\sum_{\mu=0}^{\nu}\Delta_{\nu-\mu}\sum_{\rho=0}^{\mu}\Omega^\rho\times\Omega^{\mu-\rho}\ . \tag{4.7}$$

The decomposition of the kernel $\mathscr{V}$ is now obtained by inserting Eqs. (2.6) into (4.1) and then using (4.3), (4.4), (4.6), and (4.7)

$$\mathscr{V}=\sum_{IJKL}\sum_{\nu=0}^{m[IJKL]}\mathscr{V}_\nu^{IJKL}\ , \tag{4.8a}$$

$$\mathscr{V}_\nu^{IJKL}=\tfrac{1}{2}\det M^{11}\det M^{22}\sum_{\mu=0}^{\nu}\Delta_{\nu-\mu}\sum_{\rho=0}^{\mu}\theta_{\rho,\mu-\rho}^{IJKL}\ . \tag{4.8b}$$

The symbols $\theta_{\rho,\mu-\rho}^{IJKL}$ denote traces of tensors which comprise a characteristic factor of type (4.5). Ten of these 16 traces are listed in Table II where the tensor V with the elements

$$V_{ijkl}^{IJKL}:=\sum_{i'}\sum_{j'}(M^{II})_{ii'}^{-1}(M^{JJ})_{jj'}^{-1}v_{i'j'kl}^{IJKL} \tag{4.9}$$

is used for abbreviation. Of course the tensor indices i, j, k, and l run within the range given by the size of the block matrices, i.e., N_I, N_J, N_K, and N_L, respectively. Owing to relations of the type

$$\omega^{21}(\Omega^{11})^\rho=(\Omega^{22})^\rho\omega^{21}\ ,$$

which follow from (2.5), the role of the matrices Ω^{11} and Ω^{22} in the tensor traces of Table II may be interchanged; we choose to write Ω^{11} whenever feasible in both Tables I and II. Of course it is advantageous to use the matrix of smaller size as often as possible.

The remaining six tensor traces with IJKL classification

2121 1121 2212

2112 2111 1222

have not been enclosed in Table II because of the obvious symmetry property

$$\mathscr{V}_\nu^{IJKL}=\mathscr{V}_\nu^{JILK}\ .$$

Moreover, if the same set of single-particle states is used in both bra and ket, the symmetry property

$$v_{ijkl}^{IJKL}(q_I'q_J',q_Kq_L)=v_{klij}^{KLIJ}(q_Kq_L,q_I'q_J')^*\ ,$$

cf. Eq. (4.2), leads to

$$\mathscr{V}_\nu^{1211}=(\mathscr{V}_\nu^{1112})^\dagger\ ,$$
$$\mathscr{V}_\nu^{2112}=(\mathscr{V}_\nu^{1221})^\dagger\ ,$$
$$\mathscr{V}_\nu^{2211}=(\mathscr{V}_\nu^{1122})^\dagger\ ;$$

this reduces the number of terms which actually have to be calculated to seven.

In order to compute the boundaries $m[IJKL]$ it is essential to use both decompositions (2.6a) and (2.6b) when deriving (4.8). A comparison of the resulting λ polynomials then gives the values listed in the third column of Table II.

We further state that due to the definition (4.5) each tensor trace can be written in the form

$$\begin{aligned}\theta_{\rho,\mu-\rho}^{IJKL}&=\mathrm{tr}[P^{KI}(\rho)\times Q^{LJ}(\mu-\rho)V]\\&={}^d\theta_{\rho,\mu-\rho}^{IJKL}-{}^p\theta_{\rho,\mu-\rho}^{IJKL}\\&=\sum_{ijkl}P_{ki}^{KI}(\rho)Q_{lj}^{LJ}(\mu-\rho)V_{ijkl}^{IJKL}\\&\quad-\sum_{ijkl}P_{ki}^{KI}(\rho)Q_{lj}^{LJ}(\mu-\rho)V_{ijlk}^{IJLK}\ ,\end{aligned} \tag{4.10a}$$

where $P^{KI}(\rho)$ and $Q^{LJ}(\mu-\rho)$ denote the block matrices given in Table II. Thus each contribution $\mathscr{V}_\nu^{IJKL}$ to the interaction kernel is quite naturally split into a "direct" part ${}^d\mathscr{V}_\nu^{IJKL}$ and a "permutation" part ${}^p\mathscr{V}_\nu^{IJLK}$ according to the first and second terms in (4.10a), respectively,

TABLE II. Traces involving two-particle operators.

$IJKL$	$\theta_{\rho,\mu-\rho}^{IJKL}$	$m[IJKL]$	${}^d(\nu)$	${}^p(\nu)$
1111	$\mathrm{tr}[(\Omega^{11})^\rho\times(\Omega^{11})^{\mu-\rho}V]$	$\min(N_1-2,N_2)$	ν	ν
2222	$\mathrm{tr}[(\Omega^{22})^\rho\times(\Omega^{22})^{\mu-\rho}V]$	$\min(N_1,N_2-2)$	ν	ν
1212	$\mathrm{tr}[(\Omega^{11})^\rho\times(\Omega^{22})^{\mu-\rho}V]$	$\min(N_1-1,N_2-1)$	ν	$\nu+1$
1221	$\mathrm{tr}[\omega^{21}(\Omega^{11})^\rho\times(\Omega^{11})^{\mu-\rho}\omega^{12}V]$	$\min(N_1-2,N_2-2)$	$\nu+2$	$\nu+1$
1112	$-\mathrm{tr}[(\Omega^{11})^\rho\times\omega^{21}(\Omega^{11})^{\mu-\rho}V]$	$\min(N_1-2,N_2-1)$	$\nu+1$	$\nu+1$
1211	$-\mathrm{tr}[(\Omega^{11})^\rho\times(\Omega^{11})^{\mu-\rho}\omega^{12}V]$	$\min(N_1-2,N_2-1)$	$\nu+1$	$\nu+1$
2221	$-\mathrm{tr}[(\Omega^{22})^\rho\times(\Omega^{11})^{\mu-\rho}\omega^{12}V]$	$\min(N_1-1,N_2-2)$	$\nu+1$	$\nu+1$
2122	$-\mathrm{tr}[(\Omega^{22})^\rho\times\omega^{21}(\Omega^{11})^{\mu-\rho}V]$	$\min(N_1-1,N_2-2)$	$\nu+1$	$\nu+1$
1122	$\mathrm{tr}[\omega^{21}(\Omega^{11})^\rho\times\omega^{21}(\Omega^{11})^{\mu-\rho}V]$	$\min(N_1-2,N_2-2)$	$\nu+2$	$\nu+2$
2211	$\mathrm{tr}[(\Omega^{11})^\rho\omega^{12}\times(\Omega^{11})^{\mu-\rho}\omega^{12}V]$	$\min(N_1-2,N_2-2)$	$\nu+2$	$\nu+2$

$$\mathcal{V}_\nu^{IJKL} = {}^d\mathcal{V}_\nu^{IJKL} - {}^p\mathcal{V}_\nu^{IJLK} . \quad (4.10b)$$

The number of exchanged particles, which can be read off the matrix structure of the traces (4.10a), is different for the direct and permutation contribution in general. The last two columns of Table II list these numbers for the kernels ${}^d\mathcal{V}_\nu^{IJKL}$ and ${}^p\mathcal{V}_\nu^{IJLK}$.

The graphs already introduced when treating norm and kinetic energy kernels can also be used to visualize the interaction kernels; we attach the symbol

to the matrix elements of the two-particle operator occurring in the direct kernels and the symbol

to the matrix elements occurring in the permutation kernels. The graphical representation of $\mathcal{V}_\nu^{IJKL}$ — in the sense explained at the end of Sec. II— is displayed in Fig. 3 for $\nu=0$ and each essential $IJKL$ combination of Table II. Note that, loosely speaking, each line ending at the bra and ket boxes for the two nuclei "exhausts" precisely one nucleon from the respective nucleus. This determines the maximum number of particles left for being "connected" by additional lines which is in accordance with the boundaries $m[IJKL]$ given in Table II. Moreover, the quantities ${}^d(\nu)$ and ${}^p(\nu)$ which are interpreted as being the number of exchanged particles between the two nuclei are in accordance with half the number of crossing solid lines running between boxes attached to different nuclei. Of course the graphs corresponding to the norm and kinetic energy kernels have similar features.

From a mathematical viewpoint, the interaction kernel $\mathcal{V}(q',q)$ is, by means of (4.8a) and (4.10b), decomposed into a sum of functions ${}^d\mathcal{V}_\nu(q',q)$ and ${}^p\mathcal{V}_\nu(q',q)$ each exhibiting a characteristic dependence on the generator coordinates q' and q'. The present technique for calculating GC kernels may serve to extract some distinct features of these functions *without* getting involved in extensive computations. For example, in the orthodox GCM,[1-3] where a two-center oscillator shell model and nucleon-nucleon (NN) interactions of Gaussian shape are used, each of the kernels ${}^d\mathcal{V}_\nu$ and ${}^p\mathcal{V}_\nu$ has the form "Gaussian multiplied by polynomial" and depends on relative mean distance generator coordinates $\vec{r}'$ and $\vec{r}$. In the Appendix we present a complete listing of the respective exponential functions

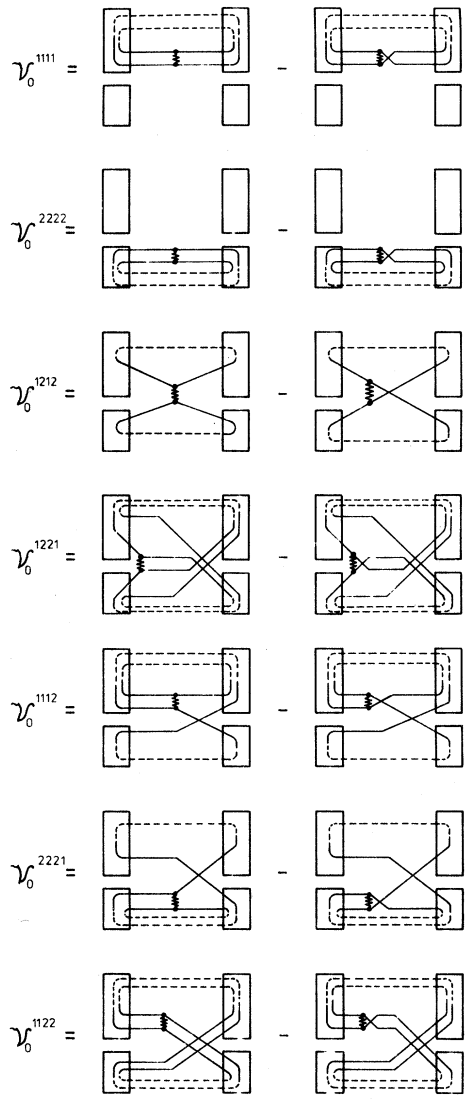

FIG. 3. Graphical illustration of the simplest contributions to the potential energy kernel.

for the general case that *different* oscillator widths in both fragments are considered.

V. SIMPLIFICATION IN CASE OF 4N-NUCLEAR STATES

The numerical extent for calculating generator coordinate kernels with the methods described in Secs. II–IV is generally reduced further if the orthogonality of single particle states with respect to spin-isospin quantum numbers is utilized. As an example we consider here the case of greatest simplification; i.e., in both fragments each orbital shell

model state is assumed to be occupied by two protons and two neutrons of opposite spin z component, respectively; thus both N_1 and N_2 being multiples of four. The overlap matrix then consists of four identical blocks, one for each spin-isospin component. Hence the norm kernel is reduced to:

$$\mathcal{N}=(\det\bar{M})^4 , \tag{5.1}$$

where $\bar{M}$ now is the overlap matrix of the single particle states with *one* fixed spin-isospin index.[18] Therefore the entire formalism of Secs. II–IV only has to be applied to $N_I/4\times N_I/4$ matrices. This turns out to be extremely simple if one of the fragments is an α particle because, in that case, the "matrix" $\bar{\Omega}^{II}$ of smaller size is just a number.

In complete analogy the kernels of one-particle operators can be written in the form[18]

$$\mathcal{T}=4(\det\bar{M})^3\mathrm{tr}[c_1^t(\bar{M})\bar{t}] , \tag{5.2}$$

where $\bar{t}$ is the matrix of the one-particle operator for one fixed spin-isospin index and $c_1(\bar{M})$ is the cofactor matrix of $\bar{M}$.

In order to treat the interaction kernel we again refer to the formulas of Brink[18] developed for the special case of $4N$ nuclei; one obtains

$$\mathcal{V}=(\det\bar{M})^2\left[X_d\sum_{\alpha\beta\gamma\delta}c_1(\bar{M})_{\alpha\beta}\,c_1(\bar{M})_{\gamma\delta}\bar{v}_{\alpha\gamma\beta\delta}-X_p\sum_{\alpha\beta\gamma\delta}c_1(\bar{M})_{\alpha\beta}\,c_1(\bar{M})_{\gamma\delta}\bar{v}_{\alpha\gamma\delta\beta}\right] . \tag{5.3}$$

Here $\bar{v}_{\alpha\gamma\beta\delta}$ denotes a potential tensor of type (4.2), where v_{op} and ϕ,ψ are only the orbital parts of the schematic (central) NN interaction[18] and the single particle states, respectively; i.e., $\alpha\beta\gamma\delta$ are pure "orbital" indices here. X_d and X_p are constants which depend on the mixing parameters of the effective interaction.[18] Application of (3.5), (3.7), (3.8), and (2.14) yields for the case of the direct traces:

$${}^d\mathcal{V}=\frac{X_d}{2}\sum_{IJKL}\sum_{\nu=0}^{\bar{m}[IJKL]}{}^d\mathcal{V}_{\nu}^{IJKL} , \tag{5.4a}$$

where

$${}^d\mathcal{V}^{IJKL}=(\det\bar{M}^{11}\det\bar{M}^{22})^4\sum_{\kappa=0}^{\bar{k}[IJKL]}\sum_{\kappa'=0}^{\bar{k}'[IJKL]}\sum_{\nu'=\max[0,\nu-(\kappa+\kappa'),\bar{n}]}^{\min[\nu-(\kappa+\kappa'),\bar{n}]}\bar{\Delta}_{\nu-(\kappa'+\kappa)-\nu'}\bar{\Delta}_{\nu'}\sum_{\lambda=0}^{\kappa}\sum_{\lambda'=0}^{\kappa'}\bar{\Delta}_{\kappa-\lambda}\bar{\Delta}_{\kappa'-\lambda'}{}^d\bar{\theta}_{\lambda,\lambda'}^{IJKL} \tag{5.4b}$$

TABLE III. Summation limits in Eq. (5.4).

$IJKL$	$\bar{m}[IJKL]$	$\bar{k}[IJKL]$	$\bar{k}'[IJKL]$
1111	$\min(N_1-2,N_2)$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}\right]$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}\right]$
2222	$\min(N_2-2,N_1)$	$\min\left[\frac{N_2}{4}-1,\frac{N_1}{4}\right]$	$\min\left[\frac{N_2}{4}-1,\frac{N_1}{4}\right]$
1212	$\min(N_1-1,N_2-1)$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}\right]$	$\min\left[\frac{N_2}{4}-1,\frac{N_1}{4}\right]$
1221	$\min(N_1-2,N_2-2)$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$
1112	$\min(N_1-2,N_2-1)$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}\right]$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$
2221	$\min(N_1-1,N_2-2)$	$\min\left[\frac{N_2}{4}-1,\frac{N_1}{4}\right]$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$
1122	$\min(N_2-2,N_1-2)$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$	$\min\left[\frac{N_1}{4}-1,\frac{N_2}{4}-1\right]$

with $\bar{n}=\frac{1}{4}\min(N_1,N_2)$. Accordingly, the contributions arising from the permutation traces can be calculated by using the same formulas (5.4), but X_d has to be replaced with X_p, ${}^d\mathcal{V}_\nu^{IJKL}$ with ${}^p\mathcal{V}_\nu^{IJKL}$, and ${}^d\bar{\theta}_{\lambda,\lambda'}^{IJKL}$ with ${}^p\bar{\theta}_{\lambda,\lambda'}^{IJKL}$. The traces $\bar{\theta}$ are formally the same as those of Table II; however, the dimensions of the corresponding tensors and matrices are reduced to a large extent. The summation limits in (5.4) are compiled in Table III.

Of course the orthogonality of the spin-isospin states can also be utilized in more complicated cases. However, the reduction of the formulas is not always as straightforward as in the case of $4N$-nuclear states. We have utilized the methods described above in the calculation of transition kernels between the α-α channel and three-body breakup channels of fragmentation $4+3+1$ in the framework of the momentum projection technique.[14] We renounce to list these kernels, since the resulting formulas[31] comprise over 30 different exponential functions, depending on three independent three dimensional parameters, cf. Eqs. (1.2). We just note that it would have been extremely tedious and time consuming to calculate these kernels entirely "by hand," but it is an easy matter to employ a computer for calculating the constants in the exponential functions for each term emerging in the systematic method described above.

VI. CONCLUDING REMARKS

As already mentioned the present method was applied to calculating kernels for the relatively light α-α system; here inelastic processes which cannot be described by currently used harmonic oscillator models could be treated in a microscopic fashion. We believe that the algorithm is apt for applications of this kind where it is inevitable to treat GC kernels depending on more than two (real) vector variables which enter from center-of-mass projection techniques. Of course the applicability to heavier systems depends on the model states under consideration; if one nucleus is a ground state α particle (or a single nucleon) all matrices involved in the algorithm have dimension 1×1 however heavy the remainder nucleus may be. Also, for heavier or more complicated systems the algorithm is efficient for calculating GCM kernels since then it is sufficient to use only $n\times n$ matrices, where n is just the particle number of the smaller fragment (or even smaller if the orthogonality of the spin-isospin states can be utilized).

The classification of the interaction kernel based on different exchange contributions $IJKL$, cf. (4.8), seems well suited to attempts such as in Ref. 32 or Ref. 25 to discuss the dynamical effect of various particle exchange contributions.[33,34] However, although the discussion in Ref. 32 may well be legitimate for high energies in Born approximation, it does not seem to be so in the whole energy range. The restriction to, say, the direct part and one distinct particle exchange contribution in the sense of Ref. 32 or 25 would not lead to a positive semidefinite norm kernel and therefore, would not appear to be very meaningful. Instead, the effect of various particle exchange contributions should be discussed in the manner of Ref. 35 where the positive semidefiniteness property of the norm kernel is reported to be maintained.

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APPENDIX: EXPONENTIAL FUNCTIONS IN GC KERNELS

Here we list all exponential functions that occur in the nuclear potential matrix elements and in the potential kernels of the generator coordinate method.[1-3] The nuclear two-body interaction is taken to be

$$V_{\rm op}(i,j)=v_0\exp\left[-\frac{1}{\gamma^2 b^2}(\vec{x}_i-\vec{x}_j)^2\right](W+BP_\sigma-HP_\tau-MP_\sigma P_\tau)\ , \tag{A1}$$

where γb is the width parameter of the Gaussian potential and P_σ and P_τ are the exchange operators for spin and isospin.[18] The GCM states are two-center oscillator shell-model states characterized by the relative distance parameters $\vec{r}$ and $\vec{r}'$ in bra and ket. We consider the general case of different oscillator widths b_1,b_2 in the respective fragments. It is convenient to define a mean width b and a relative width difference δ by

$$b^2:=\tfrac{1}{2}(b_1^2+b_2^2),\quad \delta:=\frac{b_1^2-b_2^2}{b_1^2+b_2^2}\ . \tag{A2}$$

If the one-particle oscillator states are characterized by the quantum numbers $\sigma\lambda\mu$ in spherical representation and by the displacement vectors $\vec{q}_I$ (generator coordinates, which are generally proportional to $\vec{r},\vec{r}'$), the potential matrix elements can be expressed in terms of reduced matrix elements which are independent of $\vec{q}$'s

$$\left\langle \sigma_i\lambda_i\mu_i \left[\frac{\vec{q}_I}{b_I}\right] \sigma_j\lambda_j\mu_j \left[\frac{\vec{q}_J}{b_J}\right] \mid v_{\rm op} \mid \sigma_k\lambda_k\mu_k \left[\frac{\vec{q}_K}{b_K}\right] \sigma_l\lambda_l\mu_l \left[\frac{\vec{q}_L}{b_L}\right] \right\rangle$$

$$= \exp\left\{\epsilon_S\left[\frac{S}{b}\right]^2 + \epsilon_R\left[\frac{R}{b}\right]^2 + \epsilon_{SR}\left[\frac{\vec{R}\cdot\vec{S}}{b^2}\right]\right\}$$

$$\times \sum_{NPM}\sum_{\Sigma\Lambda M'} \left[\frac{R}{b}\right]^{2N+P} Y_{PM}(\hat{\vec{R}}) \left[\frac{S}{b}\right]^{2\Sigma+\Lambda} Y_{\Lambda M'}(\hat{\vec{S}}) \sum_{\theta'\vartheta'}\sum_{\theta\vartheta}\sum_{a\alpha} (-)^{\vartheta} \begin{bmatrix} \lambda_i & \lambda_j & \theta' \\ \mu_i & \mu_j & -\vartheta' \end{bmatrix} \begin{bmatrix} \theta' & a & \theta \\ -\vartheta' & \alpha & -\vartheta \end{bmatrix}$$

$$\times \begin{bmatrix} \theta & \lambda_K & \lambda_L \\ -\vartheta & \mu_K & \mu_L \end{bmatrix} \begin{bmatrix} P & \Lambda & a \\ M & M' & -\alpha \end{bmatrix}$$

$$\times \langle \sigma_i\lambda_i\sigma_j\lambda_j\theta' \mid V^{a[IJKL]}_{NP,\Sigma\Lambda} \mid \sigma_k\lambda_k\sigma_l\lambda_l\theta \rangle \ , \tag{A3}$$

where we have used the symmetric coordinates:

$$\vec{R} = \frac{1}{\sqrt{2}}(\vec{r}+\vec{r}'), \quad \vec{S} = \frac{1}{\sqrt{2}}(\vec{r}-\vec{r}') \ . \tag{A4}$$

The sums over NPM and $\Sigma\Lambda M'$ in (A3) are all finite: The upper summation limits depend on the occupied shells in the fragments. In Table IV the parameters ϵ_R, ϵ_S, and ϵ_{SR} in the exponential functions of Eq. (A3)

TABLE IV. Parameters in the exponential functions of the potential energy matrix elements.

$IJPQ$	ϵ_S	ϵ_R	ϵ_{SR}
1111	$-\frac{1}{4}\frac{(1-n)^2}{1+\delta}$	0	0
2222	$-\frac{1}{4}\frac{(1+n)^2}{1-\delta}$	0	0
1212	$-\frac{1}{8}\left[\frac{(1-n)^2}{1+\delta}+\frac{(1+n)^2}{1-\delta}\right]$	$-\frac{1}{4}\frac{1}{1+\gamma^2/2}$	0
1112	$-\frac{n^2}{8}-\frac{1}{8}\frac{(1-n)^2}{1+\delta}-\frac{1}{16}\frac{(1+n\delta)^2}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$	$-\frac{1}{8}-\frac{1}{16}\frac{(1+\delta)^2}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$	$-\frac{n}{4}-\frac{1}{8}\frac{(1+n\delta)(1+\delta)}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$
2221	$-\frac{n^2}{8}-\frac{1}{8}\frac{(1+n)^2}{1-\delta}-\frac{1}{16}\frac{(1+n\delta)^2}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$	$-\frac{1}{8}-\frac{1}{16}\frac{(1-\delta)^2}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$	$\frac{n}{4}-\frac{1}{8}\frac{(1+n\delta)(1-\delta)}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$
1122	$-\frac{n^2}{4}$	$-\frac{1}{4}$	$-\frac{n}{2}$
1221	$-\frac{n^2}{4}-\frac{1}{4}\frac{(1+n\delta)^2}{(1-\delta^2)+\frac{\gamma^2}{2}}$	$-\frac{1}{4}$	0

TABLE V. Parameters in the exponential functions of the potential energy GCM kernels.

IJPQ	w_S	w_R	w_{SR}
1111	$-f(\nu)$	$-\frac{\nu}{4}$	0
2222	$-f(\nu)$	$-\frac{\nu}{4}$	0
1212	$-f(\nu)$	$-\frac{\nu}{4}-\frac{1}{4}\frac{1}{1+\frac{\gamma^2}{2}}$	0
1112	$-f(\nu+1)-\frac{1}{16}\frac{(1+n\delta)^2}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$	$-\frac{\nu+1}{4}-\frac{1}{16}\frac{(1+\delta)^2}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$	$-\frac{1}{8}\frac{(1+n\delta)(1+\delta)}{\left[1-\frac{\delta}{2}\right](1+\delta)+\frac{\gamma^2}{2}}$
2221	$-f(\nu+1)-\frac{1}{16}\frac{(1+n\delta)^2}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$	$-\frac{\nu+1}{4}-\frac{1}{16}\frac{(1-\delta)^2}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$	$-\frac{1}{8}\frac{(1+n\delta)(1-\delta)}{\left[1+\frac{\delta}{2}\right](1-\delta)+\frac{\gamma^2}{2}}$
1122	$-f(\nu+2)$	$-\frac{\nu+2}{4}$	0
1221	$-f(\nu+2)-\frac{1}{4}\frac{(1+n\delta)^2}{1-\delta^2+\frac{\gamma^2}{2}}$	$-\frac{\nu+2}{4}$	0

are listed. Here the abbreviation

$$n=\frac{N_1-N_2}{N_1+N_2}$$

has been used, N_1 and N_2 being the particle numbers of the respective fragments. Using Eqs. (4.8) and Table II the traces can be shown to have the following general form (only spherical fragments are considered):

$$ {}^d\mathcal{Y}_\nu^{IJKL}=\exp\left\{w_S\left[\frac{S}{b}\right]^2+w_R\left[\frac{R}{b}\right]^2+w_{SR}\left[\frac{\vec{R}\cdot\vec{S}}{b^2}\right]\right\}\sum_{\Sigma\sigma,\lambda}\left[\frac{R}{b}\right]^{\lambda+2\Sigma}\left[\frac{S}{b}\right]^{\lambda+2\sigma}P_\lambda(\hat{\vec{R}}\cdot\hat{\vec{S}})[{}^dU_\nu^{IJKL}]^{\Sigma\sigma,\lambda}, \tag{A5}$$

where P_λ denotes a Legendre polynomial. Again the summations over $\Sigma\sigma,\lambda$ are finite and the coefficients $[{}^dU_\nu^{IJKL}]^{\Sigma\sigma,\lambda}$ do not depend on $\vec{S}$, $\vec{R}$. The parameters w_S, w_R, and w_{SR} which still depend on the tupel *IJKL* are listed[36] in Table V, where the abbreviation

$$f(\nu)=\frac{1}{4}\frac{(1-n\delta)}{1-\delta^2}\left[\frac{N_1+N_2}{2}(1-n^2)-\nu(1-n\delta)\right] \tag{A6}$$

is used. For the permutation contributions ${}^p\mathcal{Y}^{IJKL}$ the same parameters w_S, w_R, and w_{SR} occur except for two cases: ${}^p\mathcal{Y}_\nu{}^{1212}$ corresponds to ${}^d\mathcal{Y}_{\nu+1}{}^{1212}$ and ${}^p\mathcal{Y}_\nu{}^{1221}$ corresponds to ${}^d\mathcal{Y}_{\nu-1}{}^{1221}$.

Finally we note that the exponential functions in the corresponding norm and kinetic energy kernels are the same as those of the interaction kernels for the case $I=J=K=L$.

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