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A New Approach to Antisymmetrization and Rearrangement in Nucleus-Nucleus Collisions

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Abstract: We report on a new microscopic model for the description of nucleus-nucleus collisions. Our method is based on a kinematical transformation to symmetrical coordinates, which at the same time describe the relative motion in all different two-body partitions of the A-nucleon system. Thereby the treatment of antisymmetrization and rearrangement collisions becomes trivial from the kinematical point of view. The fully antisymmetrized Schroedinger equation for nucleus-nucleus scattering is explicitly transformed to symmetrical coordinates. It contains no non-local potentials for the relative motion even in the region of deep interpenetration and provides a basis for the application of the two center shell model (TCSM) to the description of nucleus-nucleus collisions. The price to be paid for this simplification is the occurrence of a coupling between relative and internal motion. Numerical estimates indicate that the effects of this coupling as well as errors inherent in the phenomenological TCSM will often be small in the outer interaction region, where quasielastic reactions proceed.
I. Introduction

Consider a system of $A$ nucleons, divided into two fragment nuclei $A_\alpha, B_\alpha$. The usual microscopic description of their relative motion employs the vector

$$\mathbf{r}_\alpha = \frac{1}{A_\alpha} \sum_{i \in A_\alpha} \mathbf{r}_i - \frac{1}{B_\alpha} \sum_{i \in B_\alpha} \mathbf{r}_i$$

which connects their mass centers. It has the advantages that the kinetic energy separates exactly into a relative and an internal part, and that the mass associated with the $r_\alpha$-motion is coordinate independent and equal to the reduced mass $m_\alpha$.

The definition of $r_\alpha$ specifies what we call a "partition" $\alpha = (A_\alpha, B_\alpha)$. It implies a certain distribution of the $A$ nucleons among the fragments, e.g. nucleons $1, \ldots, A_\alpha$ making up $A_\alpha$. In contrast to this, because of the identity of nucleons, actual physical states are always "fragmentations" $a = (A_\alpha, B_\alpha)$; i.e. only the nature of the fragments is specified.

Describing physical states in terms of partitions is unnecessarily detailed and leads to well known complications. $r_\alpha$ being defined differently for different partitions, antisymmetrization introduces non-local interactions. The interaction kernel contains as many terms as there are different partitions in a fragmentation, i.e. $A!/A_\alpha!B_\alpha!$ terms. This gives 70 terms already in the case of $\alpha + \alpha$-scattering, which is still feasible, but becomes completely impractical for heavier systems. Also, the description
of rearrangement collisions is difficult, because different relative motion coordinates are involved.

While there are approximate ways to deal with these difficulties we set out to avoid them altogether. To do this one must introduce relative motion coordinates which apply directly to physical states, i.e. fragmentations. These coordinates must then be symmetrical with respect to nucleon permutations. They would not contain any reference to a specific partition of the A-nucleon system. From this we conclude that, if such coordinates do indeed exist, they would be applicable to describe the relative motion in all rearrangement channels simultaneously.

In the phenomenological two center shell model (TCSM)²,⁶⁻¹⁰ one describes relative motion with the vector $\mathbf{R}$ joining the potential centers. $R$ is a mere parameter of the model and does not depend upon any nucleon coordinates. The TCSM gives a local interaction potential. However, the use of $\mathbf{R} = (R\Theta\Phi)$ as relative motion coordinates is made in an ad hoc fashion and has no basis in scattering theory. The application of the TCSM has been restricted to elastic scattering so far, because one does not know how to relate the separation parameters for different fragmentations.

It is the aim of this paper to provide a basis for the application of the TCSM to quasielastic (rearrangement) reactions.
II. Kinematical Transformation.

1. Symmetrical Relative Motion Coordinates.

The most general coordinates which depend upon the nucleon indices in a symmetrical and linear way are the center of mass coordinates of the A-nucleon system. Therefore the desired coordinates are necessarily non-linear functions of the laboratory coordinates. Thus, in general, coordinate dependent masses will be associated with them.

Symmetrical relative motion coordinates can be defined on the basis of the quadrupole tensor \( Q_{\gamma \delta} = \sum_{i=1}^{A} x_i \cdot x_{i \gamma} \delta \).

Here \( x_i = r_i \cdot e_{\gamma} \) (\( \gamma = x, y, z \)) are the nucleon coordinates referred to a cm-frame \( e_x, e_y, e_z \), which we treat as independent coordinates for convenience.

The principal axis of \( Q \) define an intrinsic coordinate frame \( e_u \) (\( u = 1, 2, 3 \)) and three Euler angles \( \Theta_u \). They are clearly invariant with respect to nucleon permutations and can be used to describe the relative angular motion of two nuclei.

In order to define a symmetrical relative distance coordinate appropriate for the fragmentation \( a = (A_a, B_a) \) note that the concept of relative distance is well defined only in the asymptotic region of well separated nuclei. The ambiguity present in the overlap region will be exploited to define a convenient distance coordinate.

Let \( R_a \) denote the distance between nuclei \( A_a \) and \( B_a \), which as yet has a
meaning only in the asymptotic region. Asymptotically one has for the intrinsic components \( x_{iu} = \xi_i \cdot e_u \) of the nucleon position vectors, taking the 3-axis to point from \( B_a \) to \( A_a \),

\[
\frac{x_{iu}}{R_a} \sim \varepsilon_{iu}^a
\]

where

\[
\varepsilon_{iu}^a = \frac{\delta_{u3}}{A} \left\{ \begin{array}{ll}
B & \text{if } i \in A_a\\
-A & \text{if } i \in B_a
\end{array} \right.
\]

Therefore

\[
Q_{33} = \frac{\sum_{i=1}^A x_{i3}^2}{m} \sim \frac{m_a}{m} R_a^2
\]

One could simply define \( R_a \) by requiring this asymptotic identity to hold throughout configuration space. It is more convenient, however, to choose a more symmetrical form, which gives the same asymptotically. We have investigated two possibilities

\[
R_a^I = \sqrt{\frac{m}{m_a} Q}
\]

\[
R_a^\Pi = \sqrt{\frac{m}{2m_a} \tilde{Q}_{33}}
\]

where \( Q = \sum_{i=1}^A x_i^2 \), \( \tilde{Q}_{33} = 2Q_{33} - Q_{11} - Q_{22} \). \( R_a \) is clearly invariant with respect to nucleon permutations.

We define the following coordinate transformation.
- 7 -

\[
\begin{align*}
\xi_{i} &= \sum_{s=1}^{3} e_{s} x_{i} \Theta_{s} x_{i} \\
\xi_{u} &= Q_{uv} = \sum_{i=1}^{A} x_{i} x_{i} \\
\xi_{i}^{I} &= Q - \frac{m_{a}}{m} R_{a}^{I} \tag{7c}
\end{align*}
\]

or, alternatively,

\[
\xi_{i}^{I} = \tilde{Q}_{33} - \frac{2m_{a}}{m} R_{a}^{II} \tag{7d}
\]

\((i = 1, \ldots, A; \; \varphi = x, y, z; \; s = 1, 2, 3; \; u = 1, 2, 3; \; u, v, \nu = 1, 2, 3 \text{ and cyclical permutations}; \; \Theta_{s} = e_{s} e_{s} \text{ is the rotation matrix.})\)

The first 3A equations express the \(x_{i} \) in terms of three Euler angles \(\Theta_{s} = \Theta_{s} \Phi_{s} \) and 3A "intrinsic" particle coordinates \(x_{iu}\). The intrinsic frame is defined by requiring the products of inertia to vanish, i.e. \(\xi_{u} = 0\). The four symmetrical relative motion coordinates \(R_{a} = (R_{a} \Phi_{a})\) are part of a redundant set of 3A+4 coordinates \((x_{iu}, R_{a})\). The four constraints existing among these coordinates are expressed as \(\xi_{c} = 0\) \((c = 1, 2, 3, 4)\). These equations could be used to eliminate 4 coordinates from the \((x_{iu}, R_{a})\), to obtain a non-redundant set. In order to apply shell model ideas, however, we want to keep all \(x_{iu}\) and give them the status of independent variables. This can be achieved with the method of spurious coordinates, as explained in refs. 11-14. If all \((x_{iu}, R_{a})\) are allowed to vary independently we will have \(\xi_{c} \neq 0\) in general. We append the \(\xi_{c}\) to the cm-coordinates \(x_{i}^{\gamma}\) and treat them as if they were true coordinates.
of the system. The constraints $\mathcal{C}_c = 0$ can be fulfilled by integrating matrix elements over $\int d\mathcal{C}_c \mathcal{S}(\mathcal{C}_c)$. Practically, this can only be achieved on the average, as will be discussed in sect. III.1.

A complication arises from the fact that the transformation eq. (7) does not have a unique inverse. There are $2^4$ different ways of labeling the principal axis in a right handed way. This ambiguity has to be met by an appropriate symmetrization of the wave function. As this is well known from the unified model of nuclear rotations it will not be further discussed here.\textsuperscript{14,15}

It is convenient to take, as part of the channel specifications, the 3-axis as the axis along which the nuclei move. Then the Euler angles correspond directly to the usual polar angles. The third Euler angle is not needed in the practically important case of axial symmetry.

The nucleonic motion may as well be described in terms of coordinates $x_{iu}'$ referred to the nuclei instead of the $x_{iu}$, which are referred to the common mass center.

$$x_{iu}' = x_{iu} - \varepsilon_{iu}^\alpha R_{\alpha}$$  \hspace{1cm} (8)

The coordinates $(x_{iu}' R_{\alpha})$ or $(x_{iu} R_{\alpha})$ offer the following advantages for a description of nucleus-nucleus scattering:

(i) The relative motion coordinates $R_{\alpha}$ commute with the antisymmetrization operator, $[\mathcal{X}_{\alpha} R_{\alpha}] = 0$. Therefore antisymmetrization becomes a trivial matter as far as
the relative motion is concerned. It generates no
non-local interactions with respect to $R_a$. It will still
affect the internal motion, however, and thereby modify
the local potential to which the $R_a$-motion is subjected.

(ii) Relative distance coordinates for different two-body
fragmentations are identical except for a trivial multi-

\[ R'_a = \sqrt{\frac{m_a}{m_b}} R_a \]  \hspace{1cm} (9)

The angular coordinates for different fragmentations are
identical. Hence the $R_a$-coordinates are well suited for
a description of rearrangement reactions.

(iii) The intrinsic coordinates $x_{iu}$ are appropriate for two
center-, the $x_{iu}'$ for one center-shell models.

(iv) If the spin states are written in terms of scalar variables
(projections onto the internal 3-axis) the Euler angles
will rotate the whole system. Then the angular momentum
associated with them will be the total angular momentum.\(^{14}\)
Therefore, no explicit coupling of orbital and internal
angular momentum will be necessary in order to achieve
a separation into JM-subspaces.
2. Hamiltonian in Symmetrical Coordinates.

In order to write down the many-body Schroedinger equation in terms of the \( (x_{i\mu},R_{\alpha}) \) -representation the potential and kinetic energies have to be transformed. Replacing \( x_{i\mu} \) by \( (x_{i\mu},R_{\alpha}) \) via eq. (7) we find for the former

\[
V(x_{i\mu},R_{\alpha}) = \frac{1}{2} \sum_{i\mu} \psi_{i\mu}^* \left( \sum_{\nu} (x_{i\mu} - x_{i\nu}) \right) \psi_{i\mu} \tag{10}
\]

The transformation of the kinetic energy is also straightforward, although somewhat tedious. The method consists in expressing the momenta \( p_{i\mu} = -i\hbar \partial / \partial x_{i\mu} \) squaring them, and summing over \( i \) and \( \mu \) in terms of derivatives with respect to the \( (x_{i\mu},R_{\alpha}) \). In the final expressions we drop terms which contain a factor \( i \xi_\alpha \) to the left and therefore would vanish upon integrating \( \int d\xi_\alpha \delta(\xi_\alpha) \). This amounts to adding spurious energies of the form \( \xi_\alpha \partial^2 / \partial \xi_\alpha^2 \), which will not altogether vanish in practical calculations, because there \( \xi_\alpha = 0 \) can only be fulfilled approximately (see sect. III.1). It is necessary, however, to obtain a Hermitean form for the radial kinetic energy, as will be shown below.

We shall merely quote the results here; details of the calculations may be found in ref.16. We obtain

\[
T = T_{\text{rad}} + T_{\text{aug}} + T_{\text{covl}} \tag{11}
\]

where

\[
T_{\text{rad}} = -\frac{\hbar^2}{2m_{\alpha}} \left[ \frac{\partial^2}{\partial R_{\alpha}^2} - \frac{1}{R_{\alpha}} \frac{\partial}{\partial R_{\alpha}} \right] + T_{\text{covl}} \tag{12}
\]
\[ T_{\text{coupl}}^I = -\frac{\hbar^2}{2m_a} \sum_{iu} c_{iu} \frac{1}{R_a} \frac{\partial}{\partial R_a} \]  

(13)

\[ c_{iu} = x_{iu} \frac{3}{\partial x_{iu}} + \frac{2}{\partial x_{iu}} x_{1i} \]  

(14)

\[ T_{\text{coupl}}^{II} = -\frac{\hbar^2}{4m_a^2} \sum_i (2c_{i3} - c_{i1} - c_{i2}) \frac{1}{R_a} \frac{3}{\partial R_a} \]  

(15)

\[ m_a^I = m_a \]  

(16)

\[ m_a^{II} = \frac{4m_a^2 R_a^{II}}{m(3Q_{33} + Q)} \]  

(17)

\[ T_{\text{aug}} + T_{\text{pert}} = \frac{1}{2} \sum_{\nu\lambda} \frac{1}{2J_{\nu\lambda}} (J_{\nu\lambda} - J_{\nu\lambda})^2 \]  

\[ + \frac{1}{2} \sum_{\nu\lambda} \frac{1}{2D_{\nu\lambda}} [N_{\nu\lambda} (J_{\nu\lambda} - J_{\nu\lambda})^2 + (J_{\nu\lambda} - J_{\nu\lambda})N_{\nu\lambda}] \]  

\[ + \sum_{\nu\mu} \frac{P_{\nu\mu}^2}{2m} - i\hbar \sum_{\nu\mu} \frac{1}{2D_{\nu\mu}} N_{\nu\mu} \]  

(18)

The various symbols are defined as follows.

\[ p_{iu} = -i\hbar \frac{\partial}{\partial x_{iu}} \]  

(19a)

\[ J_{\nu\lambda} = \sum_i (x_{iu} p_{iu} - x_{iu} P_{iu}) \]  

(19b)

\[ \tilde{J}_{\nu\lambda} = \frac{m}{2} \frac{Q_{\nu\lambda} - Q_{\nu\lambda}}{(Q_{\nu\lambda} + Q_{\nu\lambda})^2} \]  

(19c)

\[ D_{\nu\lambda} = m \frac{Q_{\nu} - Q_{\nu}}{Q_{\nu} + Q_{\nu}} \]  

(19d)

\[ N_{\nu\lambda} = \sum_i (x_{iu} P_{iu} + x_{iu} p_{iu}) \]  

(19e)

\[ J_{\nu\lambda} \] are the components of the operator of total angular momentum, expressed in terms of Euler angles.
If one employs the primed particle coordinates, eq. (8), one gets an additional term, which is identical to $T_{\text{rad}}$ except for the sign and for $\partial/\partial R_a$ everywhere replaced by $\partial/\partial x_3^i = \sum \epsilon_{i3}^x \partial/\partial x_{iu}^i$ (here $x_{iu}^i = (m/m)^{\epsilon_{i3}^x} \sum \epsilon_{i3}^x x_{iu}^i$).

In $T_{\text{ang}} + T_{\text{part}}$, $x_{iu}^i$ then has to be replaced by $x_{iu}^i + \epsilon_{iu}^x R_a$, except in derivatives.

$T_{\text{ang}} + T_{\text{part}}$ contains the (total) angular and (intrinsic) nucleonic motion as well as couplings between the two. It is identical to the kinetic energy obtained in the unified theory of nuclear rotations. This operator has been extensively discussed by Villars and Cooper, and the reader is referred to their paper, ref. 14. The treatment of Villars and Cooper, although only intended to describe rotations of a deformed nucleus, fully applies to the angular motion of two colliding nuclei. We should point out, however, that the last term of $T_{\text{ang}} + T_{\text{part}}$ has been omitted in refs. 11, 14 and was given in ref. 12 with the wrong sign.

In what follows we shall focus our attention on the radial kinetic energy. Note the remarkable fact that the mass associated with the radial motion turns out to be completely coordinate independent for transformation I, although it was not especially designed to achieve this very convenient property. The radial mass is coordinate dependent for transformation II, as was to be generally expected for non-linear transformations.

There appears a coupling between radial and nucleonic motion. $T_{\text{coupl}}$ has the same form for primed and unprimed internal motion coordinates.
As \( x_{iu} R_a \sim \xi_{iu} \), \( x_{iu} R_a \sim 0 \) in the "important" regions of configuration space (where the particle wave functions have non-negligible amplitudes) the content of the coupling appears to be different in both cases. In ref. 16 it is shown, however, that the coupling term for the unprimed coordinates may be decomposed into a term identical to the primed coupling plus a term which in fact acts entirely on the particle coordinates. Hence the coupling always refers to the centers at \((B_a / A) R_a\) and \(-(A_a / A) R_a\).

The particle part of the coupling operator may be expressed in terms of the usual phonon creation and annihilation operators of the harmonic oscillator.

\[
C_{iu} = \alpha_{iu}^2 - \alpha_{iu}^+ \tag{20}
\]

Hence the coupling connects states differing by \( \pm 2 \) oscillator phonons. We shall discuss it further in sect. III.2.

It may come somewhat unexpectedly that the radial part of the kinetic energy does not take on the form \( \frac{\partial^2}{\partial R_a^2} + \left(\frac{2}{R_a}\right) \frac{\partial}{\partial R_a} \) as in ordinary 3-dimensional space. This can be understood from the fact that the volume element in \((x_{iu} R_a)\)-space does not equal \( dx_i dQ_a dR_a R_a^2 \). Calculating the Jacobian \( J \) of the coordinate transformation \((x_{iu} R_a) \rightarrow (x_{iu} R_a)\) in a straightforward way we find instead

\[
d\tau = d|x_i| dR_a J \delta_c = \frac{m_a}{m} d|x_i| d\Omega_a dR_a R_a (Q_{iu} - Q_{iu}) (Q_{iu} - Q_{iu}) (Q_{iu} - Q_{iu}) \delta_c \cdot \left\{ \begin{array}{ll} \frac{2}{4} & \text{(I)} \\ \frac{1}{4} & \text{(II)} \end{array} \right. \tag{21}
\]

It has the same form for the \((x_{iu} R_a)\)-coordinates.
Using this volume element we find that \( T_{\text{rad}} \) is not separately a Hermitean operator, although the complete \( T \) certainly is. The latter can be seen immediately if the Hermitean property of \( T(x^\mu, \partial/\partial x^\mu) \) is written down

\[
\int dx^\mu d\xi \delta(\xi) \not T \Phi = \int dx^\mu d\xi \delta(\xi) (T \not \Phi) \Phi
\]

and this equation transformed to the \((x, R)\)-representation.

We wish to treat the \( x^\mu \) as Cartesian coordinates and the \( R^a \) as spherical components of a vector. This can be achieved by the following transformation of the volume element.

\[
d\tau \rightarrow d\tilde\tau = dx^\mu dR^a R^a
\]

using the identity

\[
\int dx^\mu dR^a \not \Phi = \int dx^\mu dR^a R^a \tilde\not \tilde\Phi
\]

\[
\tilde\xi = \left( \frac{\not \tau}{R^a} \right)^{1/2} \not \Phi
\]

\[
\tilde\tau = \left( \frac{\not \tau}{R^a} \right)^{1/2} T \left( \frac{\not \tau}{R^a} \right)^{-1/2}
\]

In order to give a meaning to \( \not \tau^{1/2} \) we replace

\[
\delta(\xi) \rightarrow \delta_\varepsilon(\xi) = \frac{\varepsilon^{-\xi^2/\varepsilon^2}}{\varepsilon^{1/2} \pi^{1/2}}
\]

with the understanding that in final expressions \( \varepsilon \rightarrow 0 \). Taking \( \varepsilon \approx 0 \) is a way of introducing approximations, as we shall discuss in sect. III.1.

Carrying out the above transformation we obtain, absorbing all terms
without derivatives with respect to $R_a$ into $T_{\text{ang}} + T_{\text{part}}$:

$$
\widetilde{T}_{\text{rad}} = \frac{P_a^2}{2m_a} + \widetilde{T}_{\text{coupl}} + \left\{ \text{terms without derivatives} \right\}
$$

where

$$
P_a = -\frac{i\hbar}{R_a} \frac{\partial}{\partial R_a} R_a
$$

$$
\widetilde{T}_{\text{coupl}}^{(I)} = -\frac{i\hbar}{4m_a} \sum_i c_{iu} \left( \frac{1}{R_a} P_a + P_a \frac{1}{R_a} \right)
$$

$$
\widetilde{T}_{\text{coupl}}^{(II)} = -\frac{i\hbar}{8m_a} \sum_i \left( 2c_{i3} - c_{i1} - c_{i2} \right) \left( \frac{1}{R_a} P_a + P_a \frac{1}{R_a} \right)
$$

$P_a$ is the usual (Hermitean) radial momentum. The operators $i\hbar c_{iu}$, hence $\widetilde{T}_{\text{coupl}}$, are also Hermitean.

The main result of our paper is contained in eqs. (27) - (30). $\widetilde{T}_{\text{rad}}$ turns out to be separately a Hermitean operator (so that $\widetilde{T} - \widetilde{T}_{\text{rad}} = \widetilde{T}_{\text{ang}} + \widetilde{T}_{\text{part}}$ has the same property). It is, except for the coupling between radial and particle motion, identical in form to the radial part of the usual 3-dimensional kinetic energy. This result was certainly not to be expected a priori. It allows to interpret the $R_a$ -motion as being a radial motion in ordinary 3-space, and hence to identify it with the radial motion in phenomenological models, such as the TCSM (see sects. III.1,3).

We should mention that the transformation eq. (25) introduces singular
terms of the form $\frac{\partial \delta(\xi_c)}{\partial x_{iu}}$ into $\tilde{T}$ which, however, operate only on the particle coordinates and give finite contributions to matrix elements. One could avoid such singular terms if in deriving $\tilde{T}$ the complete $T$ were used without explicitly making use of the constraint equations $\xi_c = 0$, since then $T$ commutes with functions of $\xi_c$. However, the radial part of $\tilde{T}$ turns out to be not in itself a Hermitian operator in this case. Instead one obtains

$$\tilde{T}_{\text{rad}} = -\frac{\hbar^2}{2ma} \left[ \frac{\partial^2}{\partial R_a^2} - \frac{\xi}{R_a} \frac{\partial}{\partial R_a} \right] + \left\{ \text{coupling terms and terms without derivatives with respect to } R_a \right\} \ (31)$$

III. Equations of Motion.

1. Coupled Equations for Relative Motion.

In order to derive coupled channel equations for relative motion we expand the scattering state $\psi$ in terms of internal motion states $\phi^{R_a}_\beta$, to be more fully specified later. Here $\beta$ denotes a partition and other channel quantum numbers. For the transformed wave function, eq. (25a), we have

$$\tilde{\psi}(x_{iu}, R_a) = \sum_\beta \tilde{\phi}^{R_a}_\beta(x_{iu}) \chi_c(R_a) \ (32)$$

where $\tilde{\phi}^{R_a}_\beta = (\delta^\prime / R_a^2)^{1/2} \phi^{R_a}_\beta$. The superscript $R_a$ denotes a possible parametric dependence of $\phi^{R_a}_\beta$ which we may allow for in the spirit of the TCSM. The physical significance of parametric dependent channels as opposed to conventional (asymptotic) channels will be further discussed in sect. III.3.
It is important to absorb the constraints $\delta^{1/2}$ appearing in $\tilde{\Sigma}$ completely into the internal motion. Whereas the $\phi$ have to be translation and rotation invariant, the $\tilde{\phi}$ then share the invariance properties of shell model states and therefore may be expanded e.g. in the TCSM. This amounts to approximating the $\delta$-functions by spurious motions (linear and rotation oscillations) contained in shell model states. They are sharply peaked functions concentrated around $\xi_c = 0$. In the case of two center oscillator functions this amounts to putting $\Xi = (m/m_\omega)^{1/2}$ asymptotically in eq. (26), which is $0.6$ fm in the case of $16_0 + 16_0$ - scattering. Physically this means that matrix elements are not taken anymore at $\xi_c = 0$, but at $\langle \xi_c \rangle_R = 0$, implying an average over a small region $\Delta \xi_c(R) = \sqrt{\langle \xi_c^2 \rangle_R - \langle \xi_c \rangle_R^2}$ around $\xi_c = 0$ ($R$ denotes the TCSM separation parameter).

Eqs. (\ref{eq:1}) then give a relation between the radial coordinate $R_a$ and the TCSM separation parameter $R$.

$$R_a^I(R) = \sqrt{\frac{m}{m_a}} \langle Q \rangle_R$$  \hspace{1cm} (33)

$$R_a^II(R) = \sqrt{\frac{m}{2m_a}} \langle \tilde{Q}_{33} \rangle_R$$  \hspace{1cm} (34)

The range of averaging is

$$\Delta R_a^I(R) = \frac{m}{2m_a R_a} \sqrt{\sum_i \left( \langle x_{i3}^4 \rangle - \langle x_{i3}^2 \rangle^2 + \langle (x_{i3}^4 + x_{i3})^2 \rangle - \langle x_{i3}^2 + x_{i3} \rangle^2 \right) \rangle_R}$$  \hspace{1cm} (35)

The equation for $\Delta R_a^I$ differs from this by a factor $1/4$ in front of the terms involving $x_{i1}$ and $x_{i2}$.

We have performed some calculations in the TCSM, the results of which are given in table 1. It is seen that $\Delta R_a \ll R_a$ except for very deep inter-penetration in case of transformation II. Also, $\Delta R_a$ varies little over the
region where quasielastic interactions take place.

Note that the radial motion, which by definition is the motion associated with the $R_a$-coordinate, goes over into deformation and compression modes for large overlap of the colliding nuclei (small $R$), as is apparent from eqs. (33), (34).

The symmetry axis of the TCSM has to be taken as the 3-axis, so that $\langle \xi u \rangle_R = 0$ ($u = 1, 2, 3$). The positive direction of the 3-axis is part of the channel specification.

An additional effect of the spurious motions arises because the spurious part of the kinetic energy vanishes only if $\xi_c = 0$ is rigorously fulfilled. Averaging over (small) non-zero $\xi_c$ introduces spurious energies into matrix elements, which for the $\xi_u$-motion are determined by the Hermitean operator (for $mQ - m_a R_a^2 = m_x \neq 0$)

$$\tilde{F}_p = -\frac{\hbar^2}{2m_a} \left[ \left( 1 - \frac{mQ}{m_a R_a^2} \right) \frac{\partial^2}{\partial R_a^2} + \frac{2}{R_a} \frac{\partial}{\partial R_a} \right]$$

$$- \frac{\hbar^2}{2(mQ - m_a R_a^2)} - \frac{\hbar^2 (3mQ + m_a R_a^2)}{8m_a^2 R_a^4} \tag{36}$$

A practical method to correct for spurious energies is presented in ref. 17.

The Schroedinger equation in terms of symmetrical redundant coordinates is written as

$$\delta \int dx_{iu} dR_a R_a^2 \tilde{H}^* (x_{iu} R_a)(\hat{H} - E) \Phi (x_{iu} R_a) = 0 \tag{37}$$
Substituting eq. (32) and carrying out the variation according to

$$\delta \tilde{T} = \sum \tilde{\Phi} \delta \chi$$

we obtain the following set of coupled equations

$$-\frac{\hbar^2}{2m_a} \left[ \frac{\partial^2}{\partial R_a^2} + \frac{2}{R_a} \frac{\partial}{\partial R_a} \right] \chi_a(R_a) + \left\{ \left( \tilde{\alpha} R_a \right| \tilde{T} + V - E \right\} \chi_a(R_a) = \sum_\beta \left( \tilde{\alpha} R_a \right| \tilde{T} + V \left| \tilde{\beta} R_a \right) \chi_\beta(R_a)$$

(39)

The round brackets indicate matrix elements of internal states at fixed $R_a$, with $\Phi_a(x_{iu}) = (x_{iu} | \tilde{\alpha} R_a)$. In the second term on the left hand side the $\partial/\partial R_a$ operators of $\tilde{T}$ act only upon the internal motion, which we have indicated with curly brackets. To simplify the writing we have assumed that the $| \tilde{\beta} R_a$ form an orthonormal set for each $R_a$.

It is seen that all terms of eqs. (39) are local with respect to $R_a$. Antisymmetrization affects only the internal motion.

One may likewise obtain effective equations for a few (quasi-)elastic channels only, using Feshbach's projection technique. The effective many-channel interactions will still in principle be non-local with respect to $R_a$, but for not too low energy a local approximation will hold because of random phases.
In order that a solution to eqs. (39) be physically interpretable as a scattering state the wave function must satisfy the boundary conditions
\[ \tilde{\Phi}(x_i, R_a) \xrightarrow{R_a \to \infty} \sum_{\beta} \Phi_{\beta}(x_i) \left( \delta_{\alpha \beta} e^{i k_a R_a \cos \Theta} + \frac{e^{i \hat{k}_a R_a}}{R_a} f_{a \beta}(\Theta \phi) \right) \]  
(40)

Here \( \alpha \) denotes the entrance channel fragmentation. The total energy of the state eq. (40) may be written
\[ E = \frac{\hbar^2 k_a^2}{2m_a} + \epsilon_a = \frac{\hbar^2 k_b^2}{2m_a} + \epsilon_b = \frac{\hbar^2 k_c^2}{2m_b} + \epsilon_b \]  
(41)

where \( \epsilon_{a,b} \) is the asymptotic internal energy in fragmentation \( a,b \), respectively. The wave number for fragmentation \( b \) is not \( k_b \) but \( k_b = \sqrt{m_a/m_b} k_c \).

Using eq. (9) we have \( \hat{k}_b R_a = k_b R_b \), as it must. The differential cross section for the transition \( a \to b \) is given by the usual expression
\[ G_{a \to b}(\Theta \phi) = \frac{k_c}{\hat{k}_a} \left| f_{a \to b}(\Theta \phi) \right|^2 \]  
(42)

To prove that indeed eq. (40) is an asymptotic solution we now show that the additional terms produced by the coupling between radial and particle motion, which appears in the \( \tilde{T} \) of eq. (39), vanish as \( 1/R_a^2 \) or faster asymptotically.

2. Coupling between Radial and Particle Motion.

The coupling is of purely kinematical origin. While this is clear from our method in general it is most obvious from the fact that, because of the coupling, eqs. (39) do not have one-channel solutions even in the complete absence of interactions.
Technically the coupling arises from the fact that internal and relative motion coordinates are not rigorously orthogonal, being connected by the constraints $\xi_c = 0$. From eqs. (7) and (8) we find for the components of the usual relative motion vector $\mathbf{r}_c$ (transformation I)

$$\tau_{d1} = -\frac{m}{m_a R_a} \sum_i x_{i1}^1 x_{i3}^1$$

$$\tau_{d2} = -\frac{m}{m_a R_a} \sum_i x_{i2}^1 x_{i3}^1$$

$$\tau_{d3} = R_a - \frac{m}{2m_a R_a} \sum_{i\mu} x_{i\mu}^1$$

in physical space ($\xi_c = 0$). The difference between $\mathbf{r}_c = \sqrt{\sum x_{\mu}^2}$ and $R_a$ becomes very small asymptotically. In the important regions of configuration space we have $x_{i\mu}^1 / R_a \sim 0$ and $R_a - r_c$ is approximately given by the ratio of the average of the rms-radii of the scattered fragments, divided by the macroscopic distance between them. The effects of this difference are never negligible, however, because it depends upon $R_a$ and vanishes as slowly as $1/R_a$. From the fact that $\tau_{d1} \neq 0$, $\tau_{d2} \neq 0$ it is seen that also the angles of $R_a$ differ from those of $r_c$. This difference vanishes as $1/R_a^2$ asymptotically.

The physical significance of the coupling is also evident from eq. (45). If two classical nuclei were in a state of free relative motion, $r_{d3}(t) = vt$, their symmetrical distance $R_a$ would approach a linear time dependence only asymptotically. Hence their internal motion, referred to coordinate
frames at \((B_a/A)R_a\) and \(-(A_a/A)R_a\), would be described in non-inertial frames. All these effects disappear if the nuclei would be shrunked to a point, \(x_{iu}'\to 0\).

The coupling is in fact an unescapable consequence of the use of symmetrical coordinates to describe the relative motion. Such coordinates must necessarily contain a residual dependence upon the internal coordinates (spatial extension) of the fragments, otherwise they would not depend upon all nucleons in a symmetrical way.

Thus it is seen that, in order to avoid the disadvantages of the \(\lambda\)-description concerning antisymmetrization and rearrangement, one must necessarily give up the advantage of a rigorous separation between internal and relative motion. Whether this will be a favourable thing to do depends upon the possibility to handle the \((x_{iu} \leftrightarrow R_a)\)-coupling. We have as yet only achieved a partial solution to this mathematical problem. It indicates that the coupling effects will be small in the physically interesting \(R_a\)-range, as will now be shown.

We shall consider transformation I and a much simplified form of eqs. (39), dropping all angular momentum terms and treating only one particle explicitly, but keeping the exact form of the coupling, eq. (29).

\[
\left[ \frac{p_a^2}{2m_a} - \frac{i\hbar}{4m_a} \sum_u C_u \left( \frac{1}{R_a} p_a + \frac{1}{R_a} \right) \right] \psi(x_u R_a) + H_{\text{part}} - E \psi(x_u R_a) = 0 \quad (46)
\]
As a further simplification the particle Hamiltonian will be assumed of oscillator form

$$H_{\text{part}} = -\frac{\hbar^2}{2m} \sum_u \frac{\partial^2}{\partial u^2} + \frac{1}{2} m \omega^2 x^2$$  \hspace{1cm} (47)

with $x^2 = \sum_u x_u^2$. The effect of the coupling, when acting upon an oscillator state $\phi_{n\ell m}$, is

$$\sum_u c_u \phi_{n\ell m} = \left[ 2x \frac{\partial}{\partial x} + 3 \right] \phi_{n\ell m} = -N_{n\ell} \phi_{n+1\ell m} + N_{n-1\ell} \phi_{n-1\ell m}$$  \hspace{1cm} (48)

where

$$N_{n\ell} = 2\sqrt{(n+1)(n+\ell+3/2)}$$  \hspace{1cm} (49)

(For transformation II the coupling is much more complicated, with $T_{\text{coupl}}^{\text{II}}$ also changing the angular momentum $\ell$.)

We shall now obtain a solution to eq. (46) in the form of an asymptotic expansion in terms of $1/R_a$. Consider a "parent" state $(e^{ik_a R_a/R_a})\phi_{n\ell m}$ which would solve eq. (46) were it not for the coupling. The required extension of the parent state can be inferred from the fact that each action of $T_{\text{coupl}}$ generates $\pm 2$ phonons and at the same time produces a factor $1/R_a$.

This suggests to look for a solution to eq. (46) in the form

$$\Psi_{n\ell m} = \frac{e^{ik_a R_a}}{R_a} \sum_{\lambda} \frac{A^\lambda_{n\ell m}}{R_a^\lambda} \phi_{n+\nu \ell m}$$  \hspace{1cm} (50)

($\lambda = 0, \ldots, \infty; -n \leq \nu \leq \infty; A^\lambda_{\nu} = 0$ if $\lambda < |\nu|$.)

This may be generalized to A particles, in which case the solution may be written in the same form, where now $\nu = (\nu_1, \ldots, \nu_A)$, and $A^\lambda_{\nu} = 0$ if $\lambda < \sum_{i=1}^A |\nu_i|$. We expect that in the general case of non-zero
angular momentum an analogous form for $\Psi$ will hold.

Substituting eq. (50) into eq. (46) we obtain an eigenvalue equation

$$E_{\nu \lambda} = \frac{\hbar^2 k_a^2}{2 m_a} + (2n + \ell + 3/2) \hbar \omega$$

and the following recursion relation for the $A_{\nu}^{\lambda}$ (here $\nu = \frac{\hbar k_a}{m_a}$)

$$\nu A_{\nu}^{\lambda} = \frac{i \nu a}{2 \omega} (1 - \lambda) A_{\nu}^{\lambda-1} + \frac{\hbar (\lambda-2)(\lambda-1)}{4 m_a \omega} A_{\nu}^{\lambda-2}$$

$$- \frac{i \nu a}{4 \omega} \left( A_{\nu-1}^{\lambda-1} N_{n+\nu-1} - A_{\nu+1}^{\lambda-1} N_{n+\nu} e^{-i \lambda \delta} \right)$$

$$+ \frac{\hbar (2\lambda-3)}{8 m_a \omega} \left( A_{\nu-1}^{\lambda-2} N_{n+\nu-1} - A_{\nu+1}^{\lambda-2} N_{n+\nu} e^{-i \lambda \delta} \right)$$

($\lambda = 0, 1, \cdots, \infty$; $-n \leq \nu \leq \infty$; $A_{\nu}^{\lambda} = 0$ if $\lambda < |\nu|$.)

It is readily seen that they are solvable in a unique way. There are $2\lambda + 1$ equations for each $\lambda$, determining the $2\lambda + 1$ coefficients $A_{0}^{\lambda}, A_{\nu}^{\lambda}, 0 < |\nu| \leq \lambda$. $A_{0}^{\lambda}$ does not occur in $\lambda$-th order, in which instead $A_{0}^{\lambda-1}$ is determined from the equation for $\nu = 0$. $A_{0}^{\lambda}$, the amplitude of the parent state, is arbitrary (non-zero, of course).

We have not yet obtained closed-form solutions for $A_{\nu}^{\lambda}$, except in a few cases.

$$A_{\nu}^{\lambda} = \left( -\frac{i \nu a}{2 \omega} \right)^{\lambda} \frac{1}{\lambda!} \sqrt{\frac{(n+\lambda)!}{n!} \frac{\Gamma(n+\ell+\lambda+3/2)}{\Gamma(n+\ell+3/2)}}$$

$$A_{\nu}^{\lambda-1} = \left( -\frac{i \nu a}{2 \omega} \right)^{\lambda-2} \frac{1}{(\lambda-1)!} \sqrt{\frac{(n+\lambda-1)!}{n!} \frac{\Gamma(n+\ell+\lambda+1/2)}{\Gamma(n+\ell+3/2)}} \cdot \left[ \frac{\hbar (\lambda-1)^2}{4 m_a \omega} \right.$$

$$- \frac{i \nu a}{4 \omega^2} (2n + \ell + \lambda + 1/2) \left] \right.$$
For $\omega \to \infty$, which corresponds to spatial extension $\to 0$, all coefficients $A_\nu^\lambda \to 0$ for $\nu \neq 0$. The same happens for $v_a \to 0$. Thus only the parent state survives in these limits, as was to be expected.

We propose to treat the coupling in an approximate fashion, retaining only the first few terms. We have explicitly evaluated coefficients $A_\nu^\lambda / R_{a b}^\lambda$ for a number of parent states, at a relative distance of 10 fm (which is supposed to be "large"). Table 2 shows that the admixtures to the parent state are small and that successive orders decrease fast.

The coupling can be avoided altogether if one goes to the approximations of the particle-core model. Then only $A' = A - p$ "core"-nucleons would be included in the definition of $R_a$ and $\xi_{ih}$, eqs. (5) — (7). The $p$ "valence"-nucleons would only be subjected to transformation eq. (7a,6), so that their motion is not kinematically coupled to $R_a$. Upon dropping all microscopic degrees of freedom of the cores from the kinetic energy one would then get rid of the $(x_{iu} \leftrightarrow R_a)$-coupling.
3. Two Center Shell Model.

Eqs. (39) (rather their effective elastic form with $V \rightarrow V + V_{\text{eff}}$) in conjunction with eq. (33) furnish a basis for the TCSM. In what follows we shall give a brief qualitative outline of the method to be followed to "derive" the TCSM.

The internal elastic motion $\tilde{\gamma}_{R_a}^d$ must be expanded in terms of TCSM-states. The real part of the complete effective interactions has to be written as a TCSM-potential plus a residual interaction. The requirement that, for each $R_a$, the residual interaction becomes as small as possible then would lead to variational equations from which the geometrical parameters of the instantaneous ($R_a$-dependent) TCSM-potential could be calculated in terms of the basic nucleon-nucleon interaction in a completely microscopic way. Also, the instantaneous occupation scheme would be determined. All parameters would depend upon the integrals of motion, $E, J, M, \Pi$. The internal elastic motion would be modified as compared to the asymptotic internal motion of the free nuclei in such a way, that the non-quasielastic channels become decoupled on the average (except, of course, for absorption). This is the usual assumption of the "never come back"-approximation. It is by no means automatically fulfilled, but is a requirement which at all determines the parametric dependence of the TCSM-potential and the internal state $\tilde{\gamma}_{R_a}^d$.

Physically, the parametric dependence of the channel states $\tilde{\gamma}_{R_a}^d$ upon $R_a$ represents what we call "interaction polarization". When two nuclei
approach each other one will not only encounter changes in the occupation scheme of single particle or quasiparticle states (inelastic excitations, transfer). Also, the individual asymptotic states themselves may change under the influence of the shell model potential of the respective approaching nucleus in a reversible way, i.e. without changes in the occupation scheme. The extent to which this occurs will depend upon the time scale involved, being 100% in the adiabatic limit and decreasing with increasing radial motion velocity.

In terms of asymptotic states of free nuclei IP (interaction polarization) will introduce virtual states off the energy shell into the elastic wave function in an $R_a$-dependent way. These states must disappear outside the interaction region. In this picture rearrangement reactions will occur between configurations which differ from the asymptotic entrance and exit channels. The states involved will be the instantaneous states, modified from the asymptotic states by the presence of the shell model potential of the respective other nucleus. The TCSM may be regarded as a natural way to parameterize the $R_a$-dependent admixture of virtual states. In fact, if properly chosen the TCSM-wave functions should contain the closed channel components of the actual scattering problem (at least an important part of them).

The specific heavy-ion effect of "interaction polarization" has been ignored in the current descriptions of transfer reactions, except that it is
accounted for to some extent by empirical optical potentials. Qualitatively, we expect that it will effectively increase both the interaction radius and the diffuseness of the interaction region. This effect will become stronger with increasing excitation of the participating states. It will shift grazing peaks forward and enhance transfer at forward angles. This is what is required to resolve some systematic discrepancies between recent DWBA-calculations and experiment. A quantitative investigation of this point, using the TCSM and the constrained Hartree-Fock model, is in progress.

IV. Conclusion.

In this paper we have attempted to provide a foundation for a unified model of scattering of complex nuclei.

The basis of our approach has been to use microscopically defined symmetric relative motion coordinates. There still remain a number of problems - coupling between internal and relative motion, spurious energies, singular effective potentials - which must be solved before one can definitely conclude that the method has been successful.

Emphasis has also been given to the use of two-center shell model ideas and in particular interaction polarization, which should be useful in more phenomenological approaches.
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Footnotes.

[1] Properly speaking, the cm-motion should be treated by the same method as we shall use for the relative motion, namely, by means of redundant coordinates and appropriate constraints. This introduces no complications, but will be omitted here to keep all expressions as simple as possible. See refs. 11 - 14 on this point.

[2] Here and in what follows we abbreviate notationally products over coordinate differentials and δ-functions by just writing one term with an appropriate multiplication index.

[3] For simplicity we have not written out the Coulomb distortion.

[4] If one starts from a "parent" state \( (e^{-ik_aR}/a)\phi_{nlm} \) one obtains a solution which asymptotically corresponds to incoming spherical waves.
All lengths are in fermi. The calculations were made for the TCSM as described in ref. 7. The potentials were chosen to be of pure oscillator form, with \( \hbar \omega = 13.00 \, \text{MeV} \) for \(^{16}O, ^{40}Ca\) and \( \hbar \omega = 10.90 \, \text{MeV} \) for \(^{40}Ca\). The spin-orbit parameter was taken as \( \lambda = 0.08 \). No spin-orbit force has been included in the calculation of \( \Delta R_a \). The numerical evaluation of \( \Delta R_a \) is more difficult for asymmetric fragmentations and has not yet been made. An approximate calculation indicates that \( \Delta R_a \) is about 50% larger for \(^{40}Ca + ^{16}O\) than it is for \(^{40}Ca + ^{40}Ca\).
Table 2: Coupling Coefficients for $^{16}_0 + ^{16}_0$ -Scattering.

| Parent state | $|\lambda^\nu|/R_a^\lambda$ for $(\lambda,\nu)$ |
|--------------|------------------------------------------|
|              | $(1,1)$ | $(1,0)$ | $(1,1)$ | $(2,2)$ | $(2,1)$ | $(3,3)$ | $(4,4)$ |
| 1s            | .094    | .115    | .0     | .0081   | .0176   | .00067  | .000055 |
| 1p            | .122    | .192    | .0     | .0124   | .0321   | .00117  | .000105 |
| 2s            | .172    | .269    | .094   | .0214   | .0586   | .00205  | .000206 |
| 1d            | .144    | .269    | .0     | .0166   | .0490   | .00173  | .000169 |
| 2p            | .203    | .346    | .122   | .0288   | .0849   | .00346  | .000379 |
| 1f            | .163    | .346    | .0     | .0208   | .0681   | .00235  | .000247 |
| 3s            | .249    | .423    | .172   | .0407   | .1235   | .00546  | .000655 |
| 2d            | .231    | .423    | .144   | .0361   | .1143   | .00471  | .000554 |
| 1g            | .180    | .423    | .0     | .0250   | .0894   | .00304  | .000340 |

Parameters: $E_{lab} = 80$ MeV ($\tilde{E} = \nu \propto \lambda$); $\hbar\omega = 13.22$ MeV; $R_a = 10$ fm.
References.

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